Full wwPDB EM Validation Report

May 14, 2025 – 03:07 AM EDT

PDB ID	:	9DH9 / pdb_00009dh9
EMDB ID	:	EMD-46860
Title	:	State-7-Post-2 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg2+
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-09-03
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

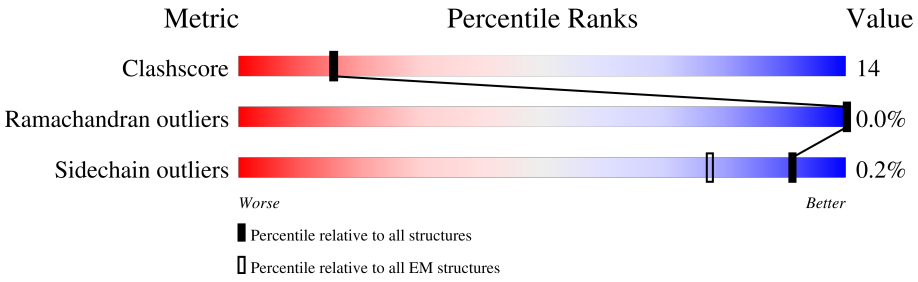
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	7% 41% 20% 38%

2 Entry composition

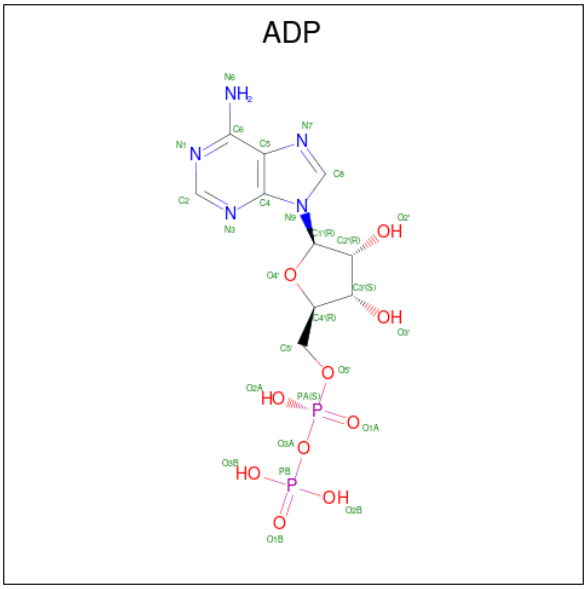
There are 5 unique types of molecules in this entry. The entry contains 23113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

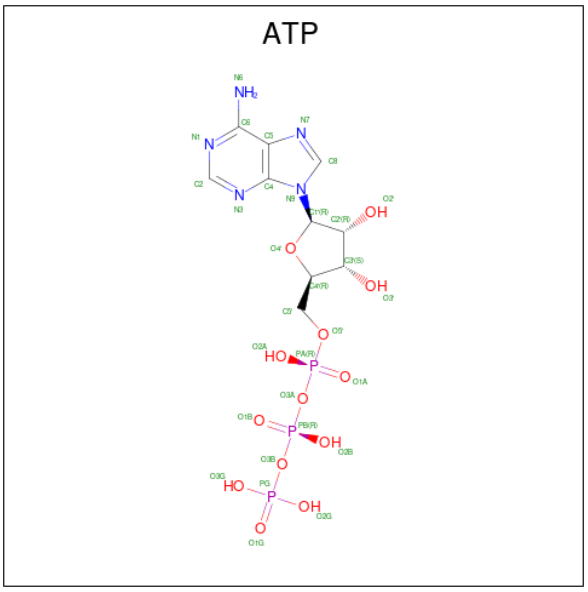
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2858	22994	14663	3967	4249	115	0	0

- 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).



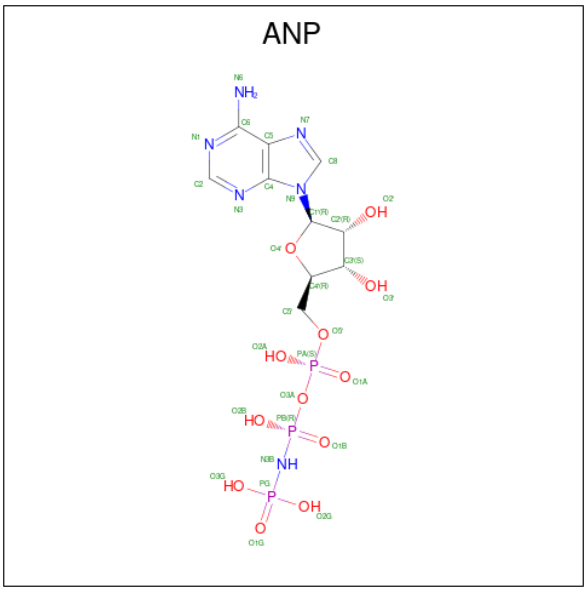
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- 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	

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

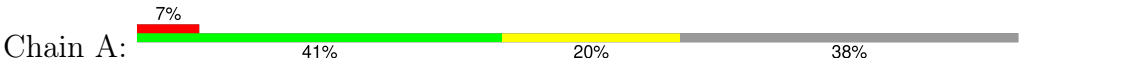
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

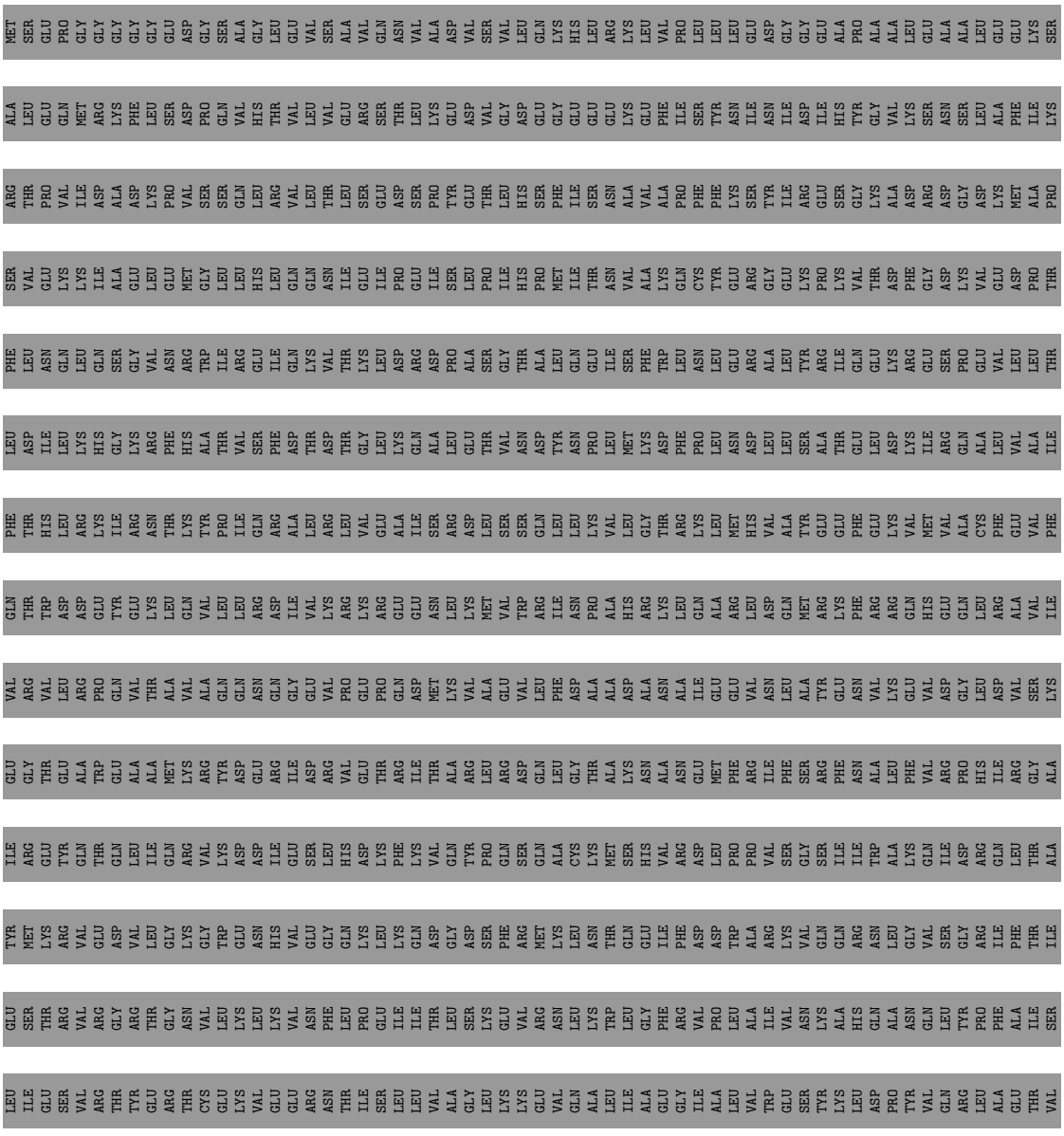
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	3	3	3	0

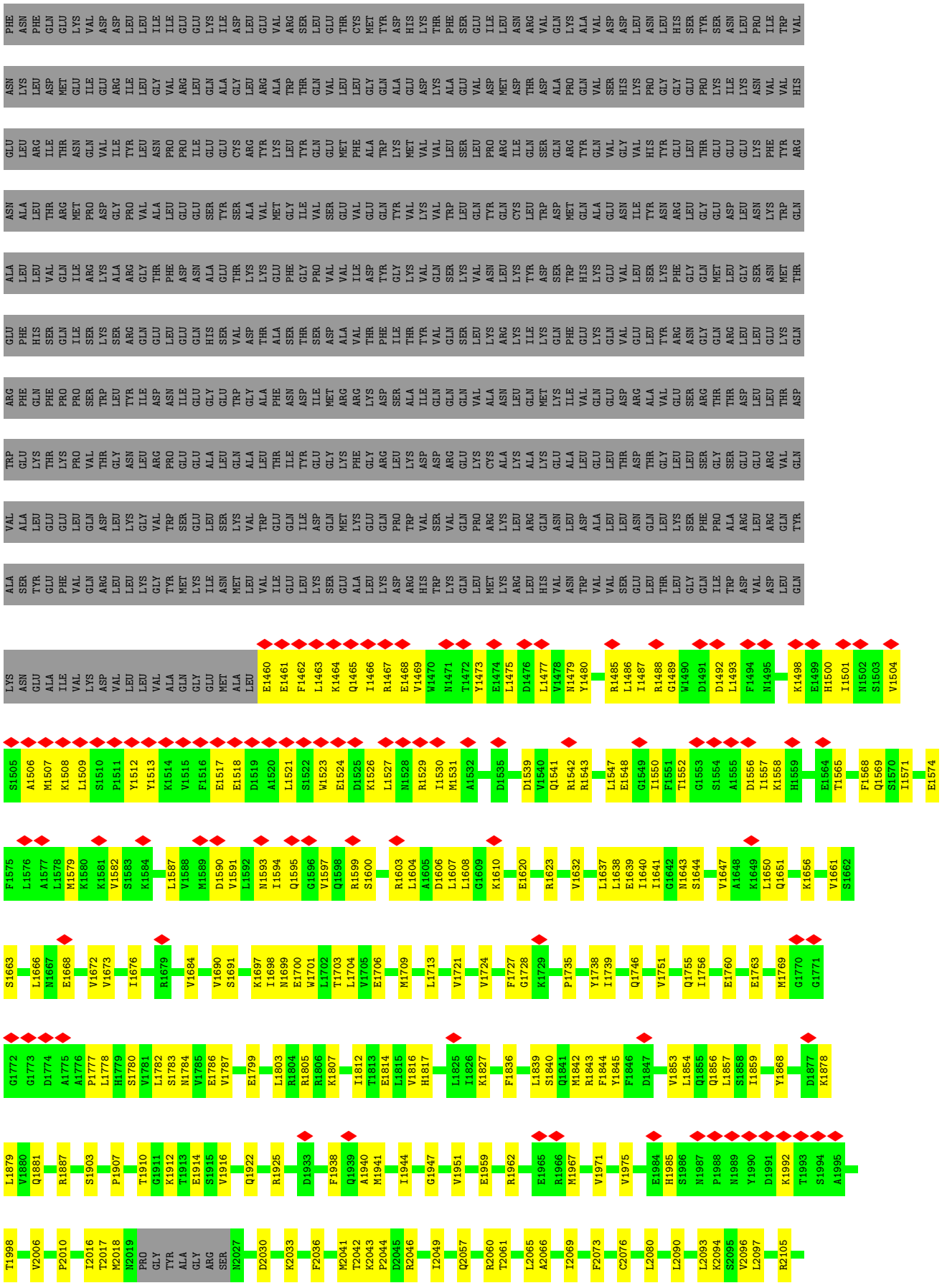
3 Residue-property plots (i)

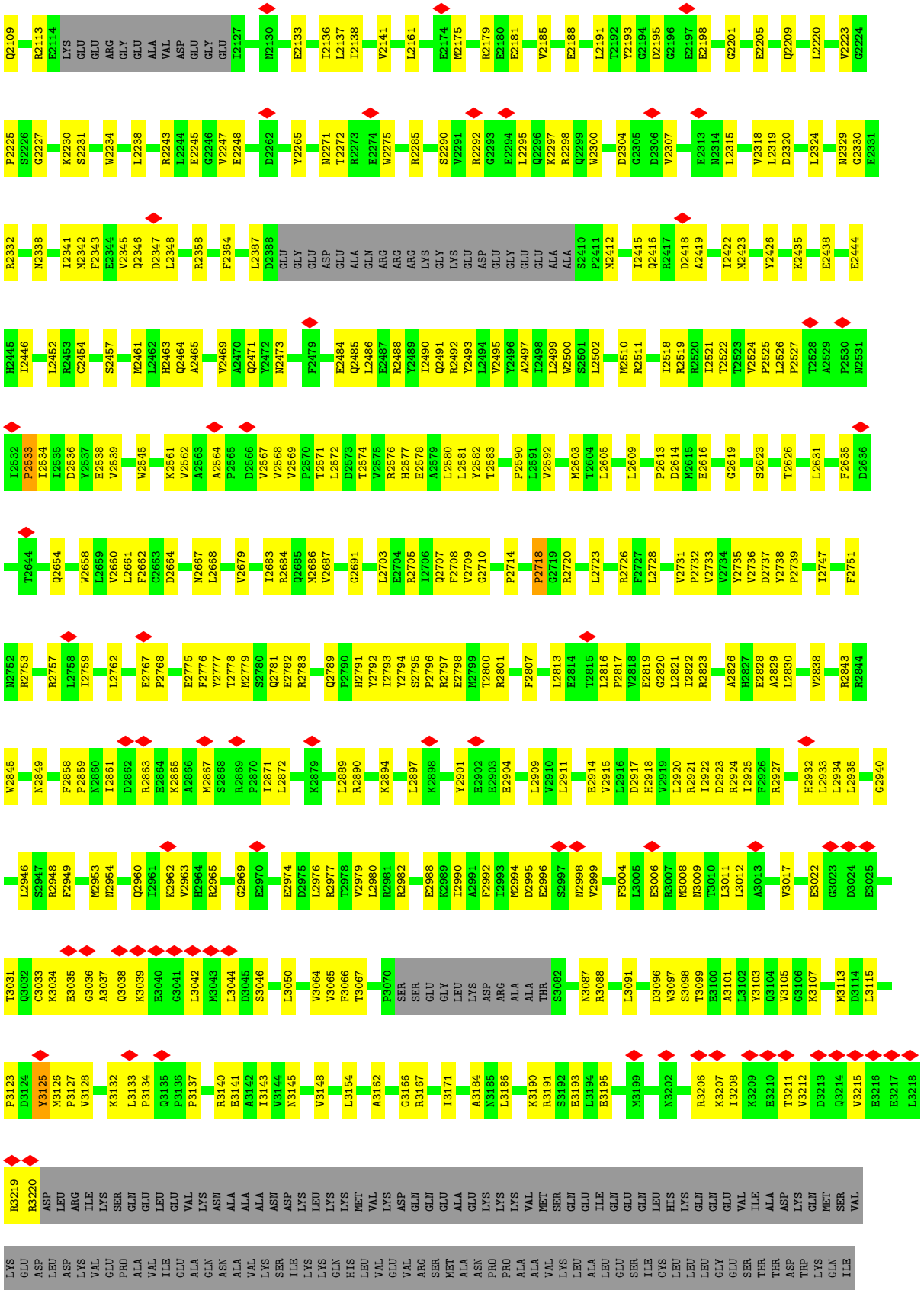
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

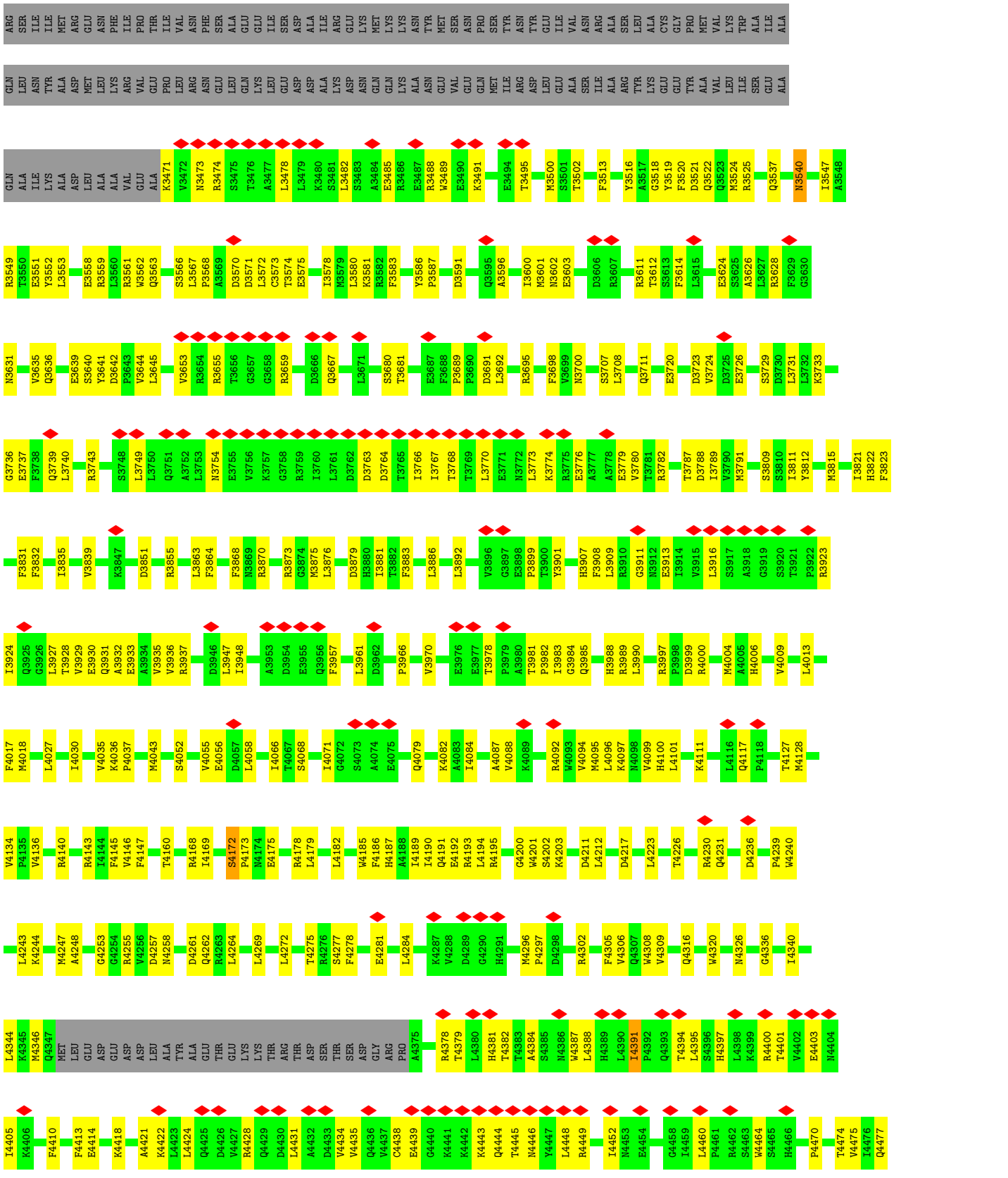
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

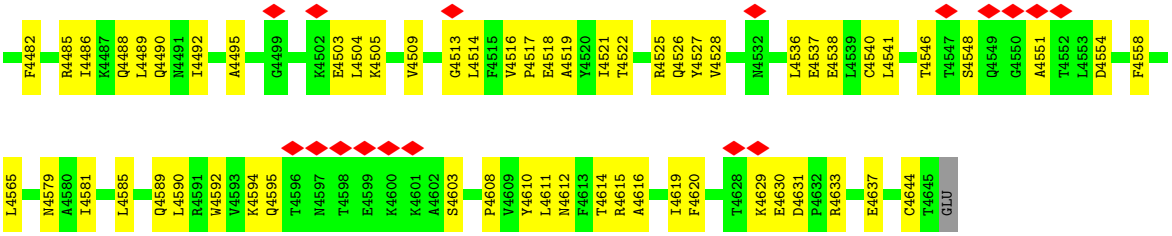







Q2109 R2113 E2114 LYS GLU GLU ARG GLY GLU ALA VAL ASP GLU GLY GLU I2127 N2130 E2133 I2136 L2137 I2138 V2141 L2161 E2174 M2175 R2179 E2180 E2181 V2185 E2188 L2191 T2192 Y2193 G2194 D2195 G2196 E2197 E2198 G2201 E2205 Q2209 L2220 V2223 G2224
P2225 S2226 G2227 K2230 S2231 W2234 L2238 R2243 L2244 E2245 G2246 V2247 E2248 D2262 Y2265 N2271 T2272 R2273 E2274 W2275 R2285 S2290 V2291 R2292 G2293 E2294 L2295 Q2296 K2297 R2298 Q2299 W2300 D2304 G2305 D2306 V2307 E2313 N2314 L2315 V2318 L2319 D2320 L2324 N2329 G2330 E2331
R2332 N2338 I2341 M2342 F2343 E2344 V2345 Q2346 D2347 L2348 R2358 F2364 L2387 D2388 GLU GLY GLU ASP GLU ALA GLN ARG ARG ARG LYS GLY LYS GLU ASP GLU GLY GLU GLU ALA ALA S2410 P2411 M2412 I2415 Q2416 R2417 D2418 A2419 I2422 M2423 Y2426 K2435 E2438 E2444
H2445 I2446 L2452 R2453 C2454 S2457 M2461 L2462 H2463 Q2464 A2465 V2469 A2470 Q2471 Y2472 N2473 F2479 E2484 Q2485 L2486 E2487 R2488 Y2489 I2490 Q2491 R2492 Y2493 L2494 V2495 Y2496 A2497 I2498 L2499 W2500 S2501 L2502 M2510 R2511 I2518 R2519 R2520 I2521 I2522 T2523 V2524 P2525 L2526 P2527 T2528 A2529 P2530 N2531
I2532 P2533 I2534 I2535 D2536 Y2537 E2538 V2539 W2545 K2561 V2562 A2563 A2564 P2565 D2566 V2567 V2568 V2569 P2570 T2571 L2572 D2573 T2574 V2575 R2576 H2577 E2578 A2579 L2580 L2581 Y2582 T2583 P2590 L2591 V2592 M2603 T2604 L2605 L2609 P2613 D2614 M2615 E2616 G2619 S2623 T2626 L2631 F2635 D2636
T2644 Q2654 W2658 L2659 V2660 L2661 F2662 C2663 D2664 N2667 L2668 V2679 I2683 R2684 Q2685 M2686 V2687 G2691 L2703 E2704 R2705 I2706 Q2707 F2708 Y2709 G2710 P2714 P2718 G2719 R2720 L2723 R2726 F2727 L2728 V2731 P2732 V2733 V2734 Y2735 V2736 D2737 Y2738 P2739 I2747 F2751
N2752 R2753 R2757 L2758 I2759 L2762 E2767 P2768 E2775 F2776 Y2777 T2778 M2779 S2780 Q2781 E2782 R2783 Q2789 P2790 H2791 Y2792 I2793 Y2794 S2795 P2796 R2797 E2798 M2799 T2800 R2801 F2807 L2813 E2814 T2815 L2816 P2817 V2818 E2819 G2820 L2821 I2822 R2823 A2826 H2827 E2828 A2829 L2830 V2838 R2843 R2844
W2845 N2849 F2858 P2859 N2860 I2861 D2862 R2863 E2864 K2865 A2866 M2867 S2868 R2869 P2870 I2871 L2872 K2879 L2889 R2890 K2894 L2897 K2898 Y2901 E2902 E2903 E2904 L2909 V2910 L2911 E2914 V2915 L2916 D2917 H2918 V2919 L2920 R2921 I2922 D2923 R2924 I2925 F2926 R2927 H2932 L2933 L2934 L2935 G2940
L2946 S2947 R2948 F2949 W2953 N2954 Q2960 I2961 K2962 V2963 H2964 R2965 G2969 E2970 E2974 D2975 L2976 R2977 T2978 V2979 L2980 R2981 R2982 E2988 K2989 I2990 A2991 F2992 I2993 M2994 D2995 E2996 S2997 N2998 V2999 F3004 L3005 E3006 R3007 M3008 N3009 T3010 L3011 L3012 A3013 V3017 E3022 G3023 D3024 E3025
T3031 Q3032 C3033 K3034 E3035 G3036 A3037 Q3038 K3039 E3040 G3041 L3042 M3043 L3044 D3045 S3046 L3050 V3064 V3065 F3066 T3067 P3070 SER SER GLU GLY LEU LYS ASP ARG ALA ALA THR S3082 N3087 R3088 L3091 D3096 W3097 S3098 T3099 E3100 A3101 L3102 Y3103 Q3104 V3105 G3106 K3107 M3113 D3114 L3115
P3123 D3124 Y3125 M3126 P3127 V3128 K3132 L3133 P3134 Q3135 P3136 P3137 R3140 E3141 A3142 I3143 V3144 N3145 V3148 L3154 A3162 G3166 R3167 I3171 A3184 N3185 L3186 K3190 R3191 S3192 E3193 L3194 E3195 M3199 N3202 R3206 K3207 I3208 K3209 E3210 T3211 V3212 D3213 Q3214 V3215 E3216 E3217 L3218
R3219 R3320 ASP LEU ARG ILE LYS SER GLN GLU LEU GLU VAL LYS ASN ALA ALA ALA ASN ASP LYS LEU LYS LYS LYS MET VAL LYS ASP GLN GLU LYS LYS LYS GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLN GLU VAL ILE ALA ASP LYS GLN MET SER VAL
LYS GLU ASP LEU ASP LYS VAL GLU PRO ALA VAL ILE GLU ALA GLN ASN ALA VAL LYS SER ILE LYS LYS GLN HIS LEU VAL GLU VAL ARG SER MET ALA ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU SER ILE CYS LEU LEU LEU GLY GLU SER THR THR ASP TRP LYS GLN ILE




F4482
R4485
I4486
K4487
Q4488
L4489
Q4490
N4491
I4492
A4495
G4499
K4502
E4503
L4504
K4505
V4509
G4513
L4514
F4515
V4516
P4517
E4518
A4519
Y4520
I4521
T4522
R4525
Q4526
Y4527
V4528
N4532
L4536
E4537
E4538
L4539
C4540
L4541
T4546
T4547
S4548
Q4549
G4550
A4551
T4552
L4553
D4554
F4558
L4565
N4579
A4580
I4581
L4585
Q4589
L4590
R4591
W4592
V4593
K4594
Q4595
T4596
N4597
T4598
E4599
K4600
K4601
A4602
S4603
P4608
Y4609
Y4610
L4611
N4612
F4613
T4614
R4615
A4616
I4619
F4620
T4628
K4629
E4630
D4631
P4632
R4633
E4637
C4644
T4645
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87075	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	1.822	Depositor
Minimum map value	-0.817	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/23487	0.45	5/31835 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2533	PRO	CA-N-CD	-7.84	101.03	112.00
1	A	2718	PRO	CA-N-CD	-5.99	103.62	112.00
1	A	3125	TYR	CA-C-N	5.68	128.55	123.10
1	A	3125	TYR	C-N-CA	5.68	128.55	123.10
1	A	2859	PRO	CA-N-CD	-5.55	104.24	112.00

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	22994	0	23053	664	0
2	A	54	0	24	5	0
3	A	31	0	12	2	0
4	A	31	0	13	4	0
5	A	3	0	0	0	0
All	All	23113	0	23102	666	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 (666) 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:3933:GLU:OE1	1:A:3937:ARG:NH1	2.03	0.92
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.54	0.88
1:A:3522:GLN:HE21	1:A:3572:LEU:HB2	1.41	0.86
1:A:2346:GLN:HB2	1:A:2726:ARG:HD3	1.58	0.85
1:A:1512:TYR:HE1	1:A:3659:ARG:HH22	1.28	0.81
1:A:1488:ARG:HE	1:A:1489:GLY:H	1.25	0.80
1:A:2992:PHE:HB3	1:A:3064:VAL:HG12	1.64	0.80
1:A:3540:ASN:O	1:A:3540:ASN:ND2	2.10	0.79
1:A:3012:LEU:HB2	1:A:3088:ARG:HD3	1.65	0.78
1:A:2795:SER:HB3	1:A:3087:ASN:HD21	1.49	0.78
1:A:2923:ASP:OD2	1:A:2927:ARG:NH2	2.17	0.78
1:A:2798:GLU:OE2	1:A:2801:ARG:NH1	2.18	0.77
1:A:2768:PRO:HB2	1:A:2858:PHE:HE1	1.48	0.77
1:A:4546:THR:HG21	1:A:4589:GLN:HE21	1.49	0.76
1:A:3835:ILE:HG12	1:A:3870:ARG:HD3	1.67	0.76
1:A:4394:THR:HA	1:A:4424:LEU:HD21	1.68	0.76
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.21	0.74
1:A:2861:ILE:HD12	1:A:2865:LYS:HD2	1.70	0.74
1:A:2863:ARG:HD2	1:A:2867:MET:HG2	1.70	0.74
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.68	0.74
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.68	0.73
1:A:3034:LYS:NZ	1:A:3044:LEU:HA	2.03	0.73
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.71	0.72
1:A:3519:TYR:HA	1:A:3700:ASN:HB2	1.71	0.72
1:A:3034:LYS:HZ3	1:A:3044:LEU:HA	1.54	0.71
1:A:4397:HIS:HE1	1:A:4421:ALA:HB3	1.54	0.71
1:A:2726:ARG:NH1	3:A:4702:ATP:O3G	2.24	0.70
1:A:2205:GLU:O	1:A:2209:GLN:HG3	1.93	0.68
1:A:3923:ARG:HH21	1:A:3948:ILE:HD12	1.58	0.68
1:A:2076:CYS:HA	1:A:2080:LEU:HD13	1.76	0.68
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.76	0.68
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.76	0.68
1:A:3720:GLU:OE1	1:A:3855:ARG:NH1	2.26	0.67
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.77	0.67
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.77	0.67
1:A:2934:LEU:HD23	1:A:3091:LEU:HG	1.77	0.67
1:A:2828:GLU:OE1	1:A:2924:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3011:LEU:HB3	1:A:3017:VAL:HG23	1.77	0.67
1:A:1746:GLN:N	1:A:1746:GLN:OE1	2.28	0.67
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.29	0.66
1:A:2616:GLU:OE2	1:A:2654:GLN:NE2	2.28	0.66
1:A:2889:LEU:HD21	1:A:2920:LEU:HD21	1.78	0.66
1:A:3822:HIS:HE1	1:A:3823:PHE:CE2	2.14	0.66
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.77	0.66
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.60	0.66
1:A:1463:LEU:HD21	1:A:1507:MET:HE1	1.78	0.65
1:A:1498:LYS:HG2	1:A:1531:MET:HE1	1.77	0.65
1:A:4281:GLU:OE2	1:A:4281:GLU:N	2.30	0.65
1:A:2925:ILE:HG21	1:A:2933:LEU:HD13	1.79	0.65
1:A:4439:GLU:OE1	1:A:4439:GLU:N	2.29	0.65
1:A:1460:GLU:N	1:A:1460:GLU:OE1	2.30	0.65
1:A:2932:HIS:CE1	1:A:3066:PHE:HB3	2.32	0.65
1:A:3984:GLY:O	1:A:3988:HIS:ND1	2.26	0.65
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.31	0.64
1:A:1461:GLU:O	1:A:1464:LYS:HG2	1.96	0.64
1:A:2776:PHE:HE1	1:A:2829:ALA:HB1	1.61	0.64
1:A:2426:TYR:OH	1:A:2491:GLN:OE1	2.15	0.64
1:A:2917:ASP:O	1:A:2921:ARG:HG3	1.98	0.64
1:A:2662:PHE:HE1	1:A:2664:ASP:HB3	1.63	0.64
1:A:2915:VAL:HG23	1:A:2946:LEU:HD11	1.80	0.64
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.80	0.64
1:A:3037:ALA:HB1	1:A:3042:LEU:HB2	1.81	0.63
1:A:4111:LYS:HE3	1:A:4111:LYS:HA	1.78	0.63
1:A:2635:PHE:HE2	1:A:2661:LEU:HD11	1.62	0.63
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.32	0.63
1:A:1547:LEU:HD13	1:A:1550:ILE:HD11	1.80	0.63
1:A:3035:GLU:O	1:A:3039:LYS:HG3	1.99	0.63
1:A:4387:TRP:O	1:A:4391:ILE:HG12	1.98	0.63
1:A:2536:ASP:OD2	1:A:2576:ARG:NH1	2.32	0.62
1:A:4169:ILE:HG21	1:A:4302:ARG:HB2	1.80	0.62
1:A:4036:LYS:HE3	1:A:4036:LYS:HA	1.80	0.62
1:A:2418:ASP:O	1:A:2422:ILE:HD12	1.99	0.62
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.31	0.62
1:A:3764:ASP:O	1:A:3768:THR:HG23	1.98	0.62
1:A:2914:GLU:OE1	1:A:2914:GLU:N	2.31	0.62
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.35	0.62
1:A:4391:ILE:HG13	1:A:4428:ARG:HH12	1.65	0.62
1:A:2897:LEU:HD21	1:A:2909:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4231:GLN:N	1:A:4231:GLN:OE1	2.31	0.62
1:A:3096:ASP:OD2	1:A:3097:TRP:N	2.33	0.61
1:A:1595:GLN:OE1	1:A:1595:GLN:N	2.32	0.61
1:A:3191:ARG:O	1:A:3195:GLU:HG2	2.01	0.61
1:A:2949:PHE:CZ	1:A:2953:MET:HE3	2.35	0.61
1:A:3547:ILE:HD11	1:A:3552:TYR:CD1	2.36	0.61
1:A:4443:LYS:HD3	1:A:4444:GLN:H	1.67	0.60
1:A:2223:VAL:HG21	1:A:2348:LEU:HD22	1.81	0.60
1:A:2933:LEU:HB3	1:A:3065:VAL:HG22	1.82	0.60
1:A:1488:ARG:HE	1:A:1489:GLY:N	1.97	0.60
1:A:2776:PHE:HA	1:A:2779:MET:SD	2.42	0.60
1:A:1812:ILE:O	1:A:1816:VAL:HG23	2.01	0.60
1:A:2935:LEU:HB2	1:A:3067:THR:HG22	1.83	0.60
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.34	0.60
1:A:2415:ILE:HD11	1:A:2473:ASN:HD22	1.67	0.59
1:A:3473:ASN:OD1	1:A:3474:ARG:N	2.35	0.59
1:A:3985:GLN:O	1:A:3989:ARG:HG3	2.01	0.59
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.02	0.59
1:A:4611:LEU:HA	1:A:4644:CYS:HB2	1.84	0.59
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.84	0.59
1:A:3628:ARG:NH1	1:A:3628:ARG:HA	2.17	0.59
1:A:4230:ARG:HD2	1:A:4230:ARG:O	2.02	0.59
1:A:1728:GLY:O	1:A:1784:ASN:ND2	2.36	0.59
1:A:1548:GLU:OE2	1:A:1552:THR:OG1	2.21	0.59
1:A:2046:ARG:HG2	1:A:2090:LEU:HD13	1.85	0.59
1:A:3927:LEU:HD13	1:A:3931:GLN:HB3	1.83	0.59
1:A:3689:PRO:HD2	1:A:3692:LEU:HB3	1.85	0.58
1:A:3628:ARG:HA	1:A:3628:ARG:HH11	1.66	0.58
1:A:2768:PRO:HB2	1:A:2858:PHE:CE1	2.35	0.58
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.36	0.58
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.36	0.58
1:A:1783:SER:O	1:A:1787:VAL:HG23	2.03	0.58
1:A:4509:VAL:HG22	1:A:4514:LEU:HD11	1.85	0.58
1:A:3729:SER:O	1:A:3733:LYS:HG3	2.04	0.58
1:A:1526:LYS:HA	1:A:1529:ARG:HE	1.68	0.58
1:A:2290:SER:OG	1:A:2295:LEU:HD23	2.04	0.58
1:A:4035:VAL:HG22	1:A:4143:ARG:HD3	1.86	0.58
1:A:2775:GLU:HG2	1:A:2779:MET:HE1	1.86	0.57
1:A:4088:VAL:HG13	1:A:4117:GLN:HE21	1.69	0.57
1:A:2592:VAL:HG22	1:A:2710:GLY:HA3	1.86	0.57
1:A:3022:GLU:N	1:A:3022:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3930:GLU:OE2	1:A:3930:GLU:N	2.35	0.57
1:A:4413:PHE:HD2	1:A:4504:LEU:HD13	1.69	0.57
1:A:4486:ILE:O	1:A:4490:GLN:HG3	2.04	0.57
1:A:1527:LEU:HA	1:A:1530:ILE:HG22	1.86	0.57
1:A:4540:CYS:HB3	1:A:4595:GLN:HG2	1.87	0.57
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.05	0.57
1:A:3641:TYR:HE1	1:A:3645:LEU:HD23	1.70	0.57
1:A:2094:LYS:HE3	2:A:4701:ADP:N3	2.20	0.57
1:A:3488:ARG:HH12	1:A:3773:LEU:HD11	1.70	0.57
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.70	0.57
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.87	0.57
1:A:4175:GLU:N	1:A:4175:GLU:OE2	2.37	0.57
1:A:2995:ASP:H	1:A:2998:ASN:HD22	1.53	0.56
1:A:1638:LEU:HD12	1:A:1641:ILE:HD11	1.86	0.56
1:A:1632:VAL:HG12	1:A:1656:LYS:HE3	1.88	0.56
1:A:2940:GLY:N	2:A:4704:ADP:O2B	2.38	0.56
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.39	0.56
1:A:3822:HIS:CE1	1:A:3823:PHE:CE2	2.93	0.56
1:A:2188:GLU:OE2	1:A:2243:ARG:NH2	2.39	0.56
1:A:4522:THR:O	1:A:4526:GLN:HG3	2.06	0.56
1:A:2049:ILE:HD13	1:A:2090:LEU:HD21	1.87	0.56
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.88	0.56
1:A:2419:ALA:O	1:A:2423:MET:HG3	2.06	0.55
1:A:2932:HIS:ND1	1:A:3064:VAL:HG23	2.21	0.55
1:A:2797:ARG:O	1:A:2801:ARG:HG3	2.06	0.55
1:A:1647:VAL:HG21	1:A:1666:LEU:HD12	1.88	0.55
1:A:1817:HIS:CE1	1:A:1881:GLN:HG2	2.42	0.55
1:A:4194:LEU:HD23	1:A:4201:TRP:CD1	2.41	0.55
1:A:2057:GLN:OE1	1:A:2105:ARG:NH2	2.39	0.55
1:A:2181:GLU:OE2	1:A:2243:ARG:HD2	2.06	0.55
1:A:2605:LEU:O	1:A:2609:LEU:HG	2.07	0.55
1:A:2737:ASP:OD1	1:A:2738:TYR:N	2.34	0.55
1:A:1751:VAL:HG11	1:A:1878:LYS:HE3	1.87	0.54
1:A:1763:GLU:OE2	1:A:1845:TYR:OH	2.22	0.54
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.07	0.54
1:A:3208:ILE:HA	1:A:3211:THR:HG22	1.88	0.54
1:A:3474:ARG:NH2	1:A:3764:ASP:H	2.05	0.54
1:A:2415:ILE:HD13	1:A:2469:VAL:HG12	1.89	0.54
1:A:2492:ARG:HH12	1:A:2525:PRO:HG2	1.72	0.54
1:A:1486:LEU:HD22	1:A:1541:GLN:HE22	1.72	0.54
1:A:3521:ASP:O	1:A:3525:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2778:THR:O	1:A:2782:GLU:HG2	2.08	0.54
1:A:3033:CYS:SG	1:A:3050:LEU:HB3	2.48	0.54
1:A:3875:MET:HE3	1:A:3879:ASP:HB3	1.90	0.54
1:A:4172:SER:HB3	1:A:4173:PRO:HD3	1.89	0.54
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.88	0.54
1:A:4027:LEU:HG	1:A:4058:LEU:HD13	1.90	0.54
1:A:4381:HIS:HB2	1:A:4438:CYS:SG	2.47	0.54
4:A:4703:ANP:O2G	4:A:4703:ANP:O1B	2.24	0.54
1:A:2030:ASP:HA	1:A:2033:LYS:HD2	1.90	0.54
1:A:3923:ARG:HG2	1:A:3924:ILE:H	1.73	0.54
1:A:4136:VAL:O	1:A:4140:ARG:HG3	2.08	0.54
1:A:2976:LEU:O	1:A:2980:LEU:HG	2.08	0.54
1:A:4391:ILE:HG13	1:A:4428:ARG:NH1	2.22	0.54
1:A:1500:HIS:O	1:A:1504:VAL:HG23	2.07	0.53
1:A:3491:LYS:O	1:A:3495:THR:HG23	2.08	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.90	0.53
1:A:1509:LEU:HD21	1:A:3624:GLU:HB3	1.89	0.53
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.72	0.53
1:A:2181:GLU:O	1:A:2185:VAL:HG23	2.07	0.53
1:A:2245:GLU:OE2	1:A:2298:ARG:NH2	2.41	0.53
1:A:1523:TRP:HA	1:A:1526:LYS:HG2	1.90	0.53
1:A:1971:VAL:O	1:A:1975:VAL:HG23	2.09	0.53
1:A:2965:ARG:HB2	1:A:3642:ASP:OD1	2.07	0.53
1:A:3763:ASP:HA	1:A:3766:ILE:HG22	1.90	0.53
1:A:1492:ASP:OD1	1:A:1493:LEU:N	2.41	0.53
1:A:2789:GLN:HE21	1:A:2838:VAL:HG21	1.73	0.53
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.91	0.53
1:A:1568:PHE:HA	1:A:1571:ILE:HG22	1.90	0.53
1:A:2271:ASN:OD1	1:A:2272:THR:N	2.41	0.53
1:A:2801:ARG:NH2	1:A:3087:ASN:O	2.37	0.53
1:A:3115:LEU:HD23	1:A:3143:ILE:HD12	1.90	0.53
1:A:3115:LEU:H	1:A:3140:ARG:HH21	1.55	0.53
1:A:3219:ARG:NH1	1:A:3220:ARG:HB2	2.24	0.53
1:A:3935:VAL:HG23	1:A:3947:LEU:HD23	1.90	0.53
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.07	0.53
1:A:2932:HIS:ND1	1:A:3064:VAL:O	2.41	0.53
1:A:3133:LEU:HB2	1:A:3134:PRO:HD3	1.91	0.53
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.24	0.53
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.89	0.53
1:A:2133:GLU:HA	1:A:2136:ILE:HD12	1.90	0.53
1:A:2412:MET:O	1:A:2416:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2932:HIS:HE1	1:A:3066:PHE:HB3	1.72	0.53
1:A:1842:MET:HE3	1:A:1922:GLN:HG2	1.92	0.52
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.91	0.52
1:A:2484:GLU:HG2	1:A:2485:GLN:N	2.24	0.52
1:A:2519:ARG:HG3	1:A:2526:LEU:HD22	1.91	0.52
1:A:3038:GLN:NE2	1:A:3042:LEU:O	2.42	0.52
1:A:4201:TRP:O	1:A:4203:LYS:N	2.41	0.52
1:A:1606:ASP:O	1:A:1610:LYS:HG2	2.09	0.52
1:A:4236:ASP:OD2	1:A:4275:THR:OG1	2.27	0.52
1:A:4394:THR:HA	1:A:4424:LEU:CD2	2.38	0.52
1:A:2329:ASN:OD1	1:A:2330:GLY:N	2.43	0.52
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.39	0.52
1:A:2753:ARG:O	1:A:2757:ARG:HG3	2.10	0.52
1:A:3519:TYR:HB2	1:A:3698:PHE:HB3	1.91	0.52
1:A:3928:THR:HG22	1:A:3929:VAL:H	1.75	0.52
1:A:4172:SER:HB3	1:A:4173:PRO:CD	2.39	0.52
1:A:4175:GLU:HG3	1:A:4278:PHE:HE2	1.75	0.52
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.10	0.52
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.33	0.52
1:A:1756:ILE:O	1:A:1760:GLU:HG3	2.10	0.51
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.91	0.51
1:A:4079:GLN:HA	1:A:4082:LYS:HE3	1.92	0.51
1:A:4187:HIS:NE2	1:A:4191:GLN:OE1	2.43	0.51
1:A:2979:VAL:HG13	1:A:2990:ILE:HG21	1.92	0.51
1:A:2982:ARG:HG2	1:A:2988:GLU:OE1	2.10	0.51
1:A:1488:ARG:NE	1:A:1489:GLY:H	2.02	0.51
1:A:2295:LEU:HA	1:A:2338:ASN:HD21	1.75	0.51
1:A:3788:ASP:OD1	1:A:3789:ILE:HD12	2.11	0.51
1:A:3932:ALA:O	1:A:3936:VAL:HG23	2.10	0.51
1:A:4565:LEU:HB2	1:A:4585:LEU:HD11	1.91	0.51
1:A:1684:VAL:HG22	1:A:1746:GLN:HE21	1.75	0.51
1:A:2265:TYR:OH	1:A:2315:LEU:HG	2.10	0.51
1:A:3580:LEU:HD23	1:A:3600:ILE:HD13	1.92	0.51
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.91	0.51
1:A:1912:LYS:HE2	1:A:2017:THR:CG2	2.41	0.51
1:A:4485:ARG:O	1:A:4489:LEU:HG	2.11	0.51
1:A:1727:PHE:HE1	1:A:1738:TYR:HA	1.76	0.51
1:A:2667:ASN:HB3	1:A:2723:LEU:HD11	1.92	0.51
1:A:2691:GLY:HA2	1:A:2703:LEU:HD13	1.93	0.51
1:A:2914:GLU:O	1:A:2918:HIS:CD2	2.64	0.51
1:A:2307:VAL:HG13	1:A:2345:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4378:ARG:HD3	1:A:4378:ARG:N	2.26	0.51
1:A:2791:HIS:HB2	1:A:3091:LEU:HD23	1.93	0.51
1:A:2500:TRP:CE3	1:A:2580:LEU:HD11	2.46	0.50
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.92	0.50
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.10	0.50
1:A:1479:ASN:OD1	1:A:1480:TYR:N	2.44	0.50
1:A:3103:TYR:CE2	1:A:3107:LYS:HE2	2.46	0.50
1:A:4202:SER:OG	1:A:4261:ASP:OD2	2.29	0.50
1:A:1782:LEU:HD22	1:A:1827:LYS:HE3	1.93	0.50
1:A:1668:GLU:OE2	1:A:1668:GLU:N	2.38	0.50
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.92	0.50
1:A:3731:LEU:HD21	1:A:3787:THR:HG23	1.93	0.50
1:A:3612:THR:HG23	1:A:3635:VAL:HG23	1.93	0.50
1:A:4443:LYS:HD3	1:A:4444:GLN:N	2.25	0.50
1:A:1466:ILE:HG22	1:A:1523:TRP:CZ3	2.47	0.50
1:A:2060:ARG:HG2	1:A:2061:THR:HG23	1.94	0.49
1:A:2533:PRO:HD2	1:A:2533:PRO:O	2.12	0.49
1:A:3206:ARG:HA	1:A:3206:ARG:NE	2.27	0.49
1:A:3474:ARG:HE	1:A:3763:ASP:HB3	1.75	0.49
1:A:3520:PHE:CD1	1:A:3524:MET:HG2	2.48	0.49
1:A:4316:GLN:HG3	1:A:4320:TRP:CE3	2.47	0.49
1:A:2444:GLU:HB2	1:A:2510:MET:HE3	1.95	0.49
1:A:2571:THR:H	1:A:2574:THR:HB	1.77	0.49
1:A:2631:LEU:HD13	1:A:2686:MET:HE1	1.95	0.49
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.78	0.49
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.53	0.49
1:A:3723:ASP:HA	1:A:3726:GLU:HG2	1.93	0.49
1:A:1907:PRO:HD2	1:A:2042:THR:HA	1.95	0.49
1:A:2315:LEU:HD13	1:A:2343:PHE:HZ	1.78	0.49
1:A:3006:GLU:HA	1:A:3009:ASN:HD22	1.77	0.49
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.94	0.49
1:A:3574:THR:O	1:A:3578:ILE:HG12	2.13	0.49
1:A:1508:LYS:HA	1:A:1513:TYR:CD1	2.48	0.49
1:A:2220:LEU:N	1:A:2341:ILE:O	2.43	0.49
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	1.95	0.49
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.13	0.49
1:A:3776:GLU:O	1:A:3780:VAL:HG23	2.12	0.49
1:A:4193:ARG:NH1	1:A:4200:GLY:O	2.46	0.49
1:A:4485:ARG:HD3	1:A:4513:GLY:O	2.12	0.49
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.95	0.49
1:A:1910:THR:HA	1:A:2044:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3821:ILE:HD11	1:A:4346:MET:HE2	1.93	0.49
1:A:4284:LEU:HD21	1:A:4296:MET:SD	2.53	0.49
1:A:4444:GLN:NE2	1:A:4449:ARG:HB2	2.28	0.49
1:A:1672:VAL:HG12	1:A:1691:SER:HA	1.95	0.49
1:A:1799:GLU:HB2	1:A:2109:GLN:NE2	2.28	0.49
1:A:2096:VAL:HG11	1:A:2141:VAL:HG22	1.95	0.49
1:A:2138:ILE:HD11	1:A:2161:LEU:HD13	1.94	0.49
1:A:2867:MET:HA	1:A:2867:MET:HE3	1.95	0.49
1:A:1799:GLU:HB2	1:A:2109:GLN:HE22	1.77	0.48
1:A:2285:ARG:HG3	1:A:2285:ARG:HH11	1.78	0.48
1:A:3128:VAL:HB	1:A:3145:ASN:OD1	2.13	0.48
1:A:1506:ALA:O	1:A:3667:GLN:NE2	2.45	0.48
1:A:2789:GLN:HB2	1:A:2792:TYR:CG	2.48	0.48
1:A:3190:LYS:HA	1:A:3193:GLU:HG2	1.95	0.48
1:A:1985:HIS:CE1	1:A:2010:PRO:HB3	2.49	0.48
1:A:3999:ASP:OD2	1:A:4000:ARG:HG2	2.14	0.48
1:A:3736:GLY:O	1:A:3740:LEU:HD23	2.13	0.48
1:A:2813:LEU:HD13	1:A:2816:LEU:HD22	1.95	0.48
1:A:3471:LYS:HB2	1:A:3474:ARG:HG2	1.94	0.48
1:A:3583:PHE:CD1	1:A:3587:PRO:HD3	2.49	0.48
1:A:3691:ASP:O	1:A:3695:ARG:HG3	2.14	0.48
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.48	0.48
1:A:4192:GLU:OE2	1:A:4195:ARG:NH2	2.46	0.48
1:A:1466:ILE:HA	1:A:1469:VAL:HG12	1.95	0.48
1:A:3154:LEU:HB3	1:A:3171:ILE:CD1	2.44	0.48
1:A:4128:MET:SD	1:A:4134:VAL:HG21	2.53	0.48
1:A:4226:THR:HG21	1:A:4239:PRO:HD3	1.94	0.48
1:A:1769:MET:HE1	1:A:1778:LEU:HG	1.96	0.48
1:A:2720:ARG:HG2	1:A:2720:ARG:HH11	1.79	0.48
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.96	0.48
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.96	0.48
1:A:4211:ASP:OD2	1:A:4255:ARG:NH1	2.46	0.48
1:A:1467:ARG:HD3	1:A:1523:TRP:HZ2	1.79	0.47
1:A:1941:MET:HE2	1:A:1941:MET:HA	1.95	0.47
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.95	0.47
1:A:3561:ARG:NH1	1:A:3603:GLU:OE1	2.44	0.47
1:A:3907:HIS:HA	1:A:3911:GLY:HA3	1.96	0.47
1:A:4017:PHE:HD2	1:A:4018:MET:HE2	1.79	0.47
1:A:4055:VAL:CG1	1:A:4095:MET:HE1	2.44	0.47
1:A:4521:ILE:O	1:A:4525:ARG:HG3	2.13	0.47
1:A:2191:LEU:HD22	3:A:4702:ATP:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2435:LYS:HA	1:A:2438:GLU:HG3	1.95	0.47
1:A:3868:PHE:HA	1:A:3883:PHE:HE2	1.79	0.47
1:A:1462:PHE:O	1:A:1466:ILE:HG12	2.14	0.47
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.14	0.47
1:A:4240:TRP:O	1:A:4244:LYS:HG3	2.14	0.47
1:A:4474:THR:HB	1:A:4477:GLN:OE1	2.14	0.47
1:A:2776:PHE:CE1	1:A:2829:ALA:HB1	2.47	0.47
1:A:2387:LEU:HD21	1:A:2463:HIS:ND1	2.30	0.47
1:A:2791:HIS:HB2	1:A:3091:LEU:CD2	2.44	0.47
1:A:2911:LEU:HD12	1:A:2915:VAL:HG13	1.97	0.47
1:A:1709:MET:O	1:A:1713:LEU:HD23	2.15	0.47
1:A:2838:VAL:O	1:A:2843:ARG:NH2	2.48	0.47
1:A:4305:PHE:O	1:A:4309:VAL:HG23	2.14	0.47
1:A:1805:ARG:HG3	1:A:1805:ARG:HH11	1.79	0.47
1:A:2492:ARG:HH22	1:A:2525:PRO:HG2	1.78	0.47
1:A:2623:SER:N	1:A:2626:THR:OG1	2.48	0.47
1:A:2826:ALA:O	1:A:2830:LEU:HD23	2.15	0.47
1:A:2994:MET:SD	1:A:3066:PHE:HB2	2.55	0.47
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.49	0.47
1:A:3923:ARG:NH1	1:A:3923:ARG:HB2	2.29	0.47
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.97	0.47
1:A:1477:LEU:HB2	1:A:1485:ARG:NH1	2.30	0.47
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.96	0.47
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.48	0.47
1:A:1925:ARG:HG2	1:A:1925:ARG:HH11	1.79	0.47
1:A:2109:GLN:OE1	1:A:2109:GLN:HA	2.15	0.47
1:A:2751:PHE:HZ	4:A:4703:ANP:H2	1.79	0.47
1:A:3642:ASP:OD2	1:A:3644:VAL:HG12	2.14	0.47
1:A:4192:GLU:CD	1:A:4316:GLN:HE22	2.21	0.47
1:A:1571:ILE:HD11	1:A:1604:LEU:HA	1.97	0.46
1:A:1600:SER:O	1:A:1604:LEU:HG	2.15	0.46
1:A:3126:MET:N	1:A:3127:PRO:HD3	2.29	0.46
1:A:4614:THR:O	1:A:4616:ALA:N	2.48	0.46
1:A:1777:PRO:O	1:A:1780:SER:OG	2.22	0.46
1:A:4100:HIS:CE1	1:A:4101:LEU:HD23	2.51	0.46
1:A:2060:ARG:NH1	1:A:2133:GLU:OE1	2.48	0.46
1:A:2275:TRP:CG	1:A:2329:ASN:HD22	2.33	0.46
1:A:2668:LEU:CD2	1:A:3006:GLU:HG3	2.45	0.46
1:A:3892:LEU:HD11	1:A:3983:ILE:HG21	1.98	0.46
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.48	0.46
1:A:3770:LEU:O	1:A:3774:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	1.98	0.46
1:A:3908:PHE:HE1	1:A:3990:LEU:HD11	1.80	0.46
1:A:4326:ASN:HD21	1:A:4581:ILE:HG23	1.81	0.46
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.97	0.46
1:A:3125:TYR:O	1:A:3126:MET:HG2	2.15	0.46
1:A:3186:LEU:HD11	1:A:3553:LEU:HD22	1.97	0.46
1:A:3916:LEU:HD12	1:A:3937:ARG:HA	1.97	0.46
1:A:3928:THR:HG22	1:A:3929:VAL:N	2.31	0.46
1:A:1487:ILE:O	1:A:2271:ASN:ND2	2.49	0.46
1:A:1527:LEU:O	1:A:1530:ILE:HG22	2.16	0.46
1:A:1542:ARG:HA	1:A:1542:ARG:HD3	1.79	0.46
1:A:1697:LYS:O	1:A:1701:TRP:HD1	1.98	0.46
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.98	0.46
1:A:4095:MET:HE2	1:A:4095:MET:HB2	1.78	0.46
1:A:2292:ARG:HB3	1:A:2292:ARG:NH1	2.31	0.46
1:A:2526:LEU:HD23	1:A:2534:ILE:HD12	1.96	0.46
1:A:2767:GLU:HB2	1:A:2768:PRO:HD3	1.97	0.46
1:A:3601:MET:HE2	1:A:3611:ARG:NH2	2.31	0.46
1:A:4516:VAL:O	1:A:4516:VAL:HG23	2.16	0.46
1:A:4631:ASP:OD1	1:A:4631:ASP:N	2.47	0.46
1:A:2577:HIS:NE2	1:A:2736:VAL:HG12	2.31	0.46
1:A:1853:VAL:HG23	1:A:1854:LEU:HD12	1.98	0.46
1:A:2718:PRO:HD2	1:A:2718:PRO:O	2.16	0.46
1:A:4608:PRO:HG2	1:A:4610:TYR:HE2	1.81	0.46
1:A:1543:ARG:HB2	1:A:1608:LEU:HD13	1.97	0.45
1:A:3207:LYS:HZ2	1:A:3754:ASN:HB2	1.81	0.45
1:A:1465:GLN:HA	1:A:1468:GLU:HG3	1.98	0.45
1:A:1844:PHE:CD2	1:A:1859:ILE:HG12	2.50	0.45
1:A:2185:VAL:HA	1:A:2188:GLU:HG2	1.98	0.45
1:A:2511:ARG:NH2	1:A:2735:TYR:O	2.48	0.45
1:A:2581:LEU:HD11	1:A:2605:LEU:HD23	1.98	0.45
1:A:4243:LEU:HB3	1:A:4247:MET:HE2	1.99	0.45
1:A:4087:ALA:HA	1:A:4092:ARG:HG2	1.97	0.45
1:A:2018:MET:HE3	1:A:2018:MET:HB3	1.79	0.45
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.82	0.45
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.49	0.45
1:A:2248:GLU:HB3	1:A:2297:LYS:HG2	1.99	0.45
1:A:2999:VAL:HA	1:A:3004:PHE:HD2	1.81	0.45
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	1.98	0.45
1:A:1513:TYR:CZ	1:A:1517:GLU:HG2	2.52	0.45
1:A:1574:GLU:OE2	1:A:1603:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1967:MET:O	1:A:1971:VAL:HG23	2.17	0.45
1:A:3036:GLY:HA2	1:A:3039:LYS:HE3	1.97	0.45
1:A:2179:ARG:HG2	1:A:2193:TYR:OH	2.16	0.45
1:A:2304:ASP:OD1	1:A:2684:ARG:NH2	2.49	0.45
1:A:3191:ARG:HE	1:A:3500:MET:CE	2.30	0.45
1:A:3551:GLU:OE2	1:A:3551:GLU:N	2.43	0.45
1:A:4192:GLU:OE2	1:A:4316:GLN:NE2	2.32	0.45
1:A:4548:SER:HB3	1:A:4551:ALA:HB2	1.99	0.45
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.17	0.45
1:A:1477:LEU:HB2	1:A:1485:ARG:HH12	1.82	0.45
1:A:2960:GLN:HB2	1:A:2962:LYS:NZ	2.32	0.45
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.51	0.45
1:A:2568:VAL:HG22	1:A:2603:MET:SD	2.56	0.45
1:A:4395:LEU:H	1:A:4395:LEU:HD23	1.81	0.45
1:A:1903:SER:HA	1:A:2016:ILE:O	2.17	0.45
1:A:1912:LYS:O	1:A:1916:VAL:HG23	2.17	0.45
1:A:3518:GLY:O	1:A:3519:TYR:HB3	2.17	0.45
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.98	0.44
1:A:3913:GLU:HG3	1:A:3913:GLU:O	2.17	0.44
1:A:3961:LEU:O	1:A:3997:ARG:HD2	2.17	0.44
1:A:4037:PRO:HB2	1:A:4117:GLN:OE1	2.17	0.44
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.99	0.44
1:A:1513:TYR:OH	1:A:1517:GLU:HG2	2.17	0.44
1:A:2225:PRO:HD2	1:A:2364:PHE:O	2.17	0.44
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.17	0.44
1:A:4052:SER:O	1:A:4056:GLU:HB2	2.18	0.44
1:A:4631:ASP:OD2	1:A:4633:ARG:NH1	2.50	0.44
4:A:4703:ANP:N3B	4:A:4703:ANP:O1A	2.49	0.44
1:A:1571:ILE:HD11	1:A:1604:LEU:HD23	1.99	0.44
1:A:1640:ILE:HG23	1:A:1650:LEU:HD21	1.99	0.44
1:A:1735:PRO:O	1:A:1739:ILE:HG12	2.17	0.44
1:A:1836:PHE:CE1	1:A:1840:SER:HB2	2.52	0.44
1:A:4518:GLU:OE2	1:A:4518:GLU:N	2.46	0.44
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.32	0.44
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.57	0.44
1:A:3739:GLN:O	1:A:3743:ARG:HG2	2.17	0.44
1:A:4516:VAL:HG23	1:A:4519:ALA:HB3	1.99	0.44
1:A:1521:LEU:HA	1:A:1524:GLU:HG2	1.99	0.44
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.17	0.44
1:A:2963:VAL:HG21	1:A:2998:ASN:HA	2.00	0.44
1:A:2982:ARG:NH1	1:A:2988:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4418:LYS:O	1:A:4422:LYS:HG2	2.18	0.44
1:A:1666:LEU:HD23	1:A:1673:VAL:HA	1.99	0.44
1:A:1703:THR:O	1:A:1706:GLU:HG2	2.18	0.44
1:A:2113:ARG:HG2	1:A:2113:ARG:O	2.17	0.44
1:A:2578:GLU:OE2	1:A:2582:TYR:OH	2.34	0.44
1:A:3474:ARG:HH21	1:A:3763:ASP:HB3	1.82	0.44
1:A:4066:ILE:HD13	1:A:4095:MET:HE2	1.99	0.44
1:A:4378:ARG:HD3	1:A:4378:ARG:H	1.82	0.44
1:A:1639:GLU:O	1:A:1643:ASN:HB2	2.17	0.44
1:A:1803:LEU:HG	1:A:1807:LYS:HE3	1.99	0.44
1:A:1857:LEU:HD23	1:A:1868:TYR:HB2	2.00	0.44
1:A:2793:ILE:HD13	1:A:3087:ASN:HB2	1.99	0.44
1:A:3764:ASP:O	1:A:3767:ILE:HG22	2.18	0.44
1:A:4614:THR:O	1:A:4614:THR:OG1	2.36	0.44
1:A:2238:LEU:HB2	1:A:2300:TRP:CZ3	2.53	0.44
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	2.00	0.44
1:A:4537:GLU:HG3	1:A:4538:GLU:HG3	1.99	0.44
1:A:4603:SER:O	1:A:4603:SER:OG	2.36	0.44
1:A:4610:TYR:CE1	1:A:4615:ARG:HB3	2.53	0.44
1:A:1604:LEU:O	1:A:1608:LEU:HG	2.18	0.43
1:A:1782:LEU:O	1:A:1786:GLU:HG2	2.17	0.43
1:A:3191:ARG:HH21	1:A:3500:MET:HE3	1.83	0.43
1:A:3478:LEU:O	1:A:3482:LEU:HD23	2.17	0.43
1:A:3540:ASN:HD22	1:A:3540:ASN:C	2.04	0.43
1:A:4431:LEU:HA	1:A:4434:VAL:HG22	1.99	0.43
1:A:2658:TRP:CD2	1:A:2705:ARG:HA	2.53	0.43
1:A:3788:ASP:HA	1:A:3791:MET:HG3	2.00	0.43
1:A:3886:LEU:HD11	1:A:4346:MET:HE3	1.99	0.43
1:A:3981:THR:O	1:A:3982:PRO:C	2.61	0.43
1:A:4413:PHE:CE2	1:A:4504:LEU:HD22	2.53	0.43
1:A:2777:TYR:CE1	1:A:2781:GLN:HG3	2.52	0.43
1:A:2845:TRP:CE2	1:A:2849:ASN:ND2	2.81	0.43
1:A:3614:PHE:HD2	1:A:3640:SER:O	2.00	0.43
1:A:3899:PRO:HG2	1:A:3901:TYR:CZ	2.53	0.43
1:A:1690:VAL:HG21	1:A:1704:LEU:HB3	2.01	0.43
1:A:3691:ASP:HB2	1:A:3695:ARG:HH12	1.84	0.43
1:A:4518:GLU:H	1:A:4518:GLU:CD	2.26	0.43
1:A:1574:GLU:OE1	1:A:1603:ARG:NH2	2.52	0.43
1:A:1755:GLN:NE2	1:A:1814:GLU:OE1	2.52	0.43
1:A:2486:LEU:O	1:A:2490:ILE:HG12	2.18	0.43
1:A:2518:ILE:HA	1:A:2521:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2736:VAL:HG23	1:A:2736:VAL:O	2.19	0.43
1:A:2923:ASP:OD1	1:A:2954:ASN:ND2	2.36	0.43
1:A:3733:LYS:HB3	1:A:3737:GLU:HB3	2.01	0.43
1:A:3966:PRO:CD	1:A:4000:ARG:HG3	2.48	0.43
1:A:4431:LEU:O	1:A:4435:VAL:HG23	2.19	0.43
1:A:4444:GLN:OE1	1:A:4449:ARG:NH2	2.39	0.43
1:A:1878:LYS:HE2	1:A:1878:LYS:HB2	1.75	0.43
1:A:2454:CYS:HB2	1:A:2502:LEU:HD12	2.00	0.43
1:A:2762:LEU:HD13	1:A:2821:LEU:HD22	2.00	0.43
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.19	0.43
1:A:4400:ARG:HH21	1:A:4405:ILE:HD11	1.84	0.43
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.00	0.43
1:A:1512:TYR:HE1	1:A:3659:ARG:NH2	2.07	0.43
1:A:3167:ARG:HG3	1:A:3519:TYR:OH	2.18	0.43
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.18	0.43
1:A:4594:LYS:HE3	1:A:4594:LYS:HB3	1.88	0.43
1:A:1853:VAL:HA	1:A:1856:GLN:HE21	1.84	0.43
1:A:1879:LEU:HD22	2:A:4701:ADP:C4	2.54	0.43
1:A:2590:PRO:HB3	1:A:2708:PHE:HB2	2.01	0.43
1:A:1590:ASP:HA	1:A:1593:ASN:OD1	2.19	0.43
1:A:2739:PRO:HD2	1:A:2796:PRO:HG3	2.01	0.43
1:A:4084:ILE:HA	1:A:4094:VAL:HG21	2.01	0.43
1:A:4193:ARG:NH1	1:A:4264:LEU:HD21	2.34	0.43
1:A:1518:GLU:H	1:A:1518:GLU:CD	2.23	0.43
1:A:2043:LYS:HE2	1:A:2043:LYS:HB3	1.93	0.43
1:A:2581:LEU:HD21	1:A:2609:LEU:HD23	2.01	0.43
1:A:2795:SER:OG	1:A:2797:ARG:HB2	2.19	0.43
1:A:3031:THR:O	1:A:3034:LYS:HB2	2.19	0.43
1:A:3103:TYR:CZ	1:A:3107:LYS:HE2	2.54	0.43
1:A:3537:GLN:OE1	1:A:3537:GLN:HA	2.19	0.43
1:A:4055:VAL:HG11	1:A:4095:MET:HE1	2.00	0.43
1:A:1547:LEU:HA	1:A:1550:ILE:HG12	2.01	0.42
1:A:2538:GLU:HG2	1:A:2539:VAL:N	2.34	0.42
1:A:3653:VAL:HG21	1:A:3655:ARG:HH12	1.84	0.42
1:A:3707:SER:O	1:A:3711:GLN:HG3	2.19	0.42
1:A:4189:ILE:O	1:A:4193:ARG:HG3	2.19	0.42
1:A:2797:ARG:HA	1:A:2800:THR:HG22	1.99	0.42
1:A:2318:VAL:HG13	1:A:2319:LEU:HD12	2.00	0.42
1:A:2590:PRO:HG2	1:A:2731:VAL:HG12	2.01	0.42
1:A:2872:LEU:HD12	1:A:2889:LEU:HD23	2.00	0.42
1:A:3212:VAL:HA	1:A:3215:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3749:LEU:HD13	1:A:3773:LEU:HD22	2.01	0.42
1:A:4043:MET:HE2	1:A:4147:PHE:HE2	1.84	0.42
1:A:4306:VAL:O	1:A:4309:VAL:N	2.52	0.42
1:A:4504:LEU:HD23	1:A:4504:LEU:HA	1.88	0.42
1:A:2065:LEU:HD23	1:A:2065:LEU:HA	1.89	0.42
1:A:3098:SER:OG	1:A:3099:THR:N	2.52	0.42
1:A:3502:THR:HG23	1:A:3502:THR:O	2.19	0.42
1:A:3558:GLU:OE2	1:A:3581:LYS:HE3	2.20	0.42
1:A:1827:LYS:HE2	1:A:1827:LYS:HB2	1.85	0.42
1:A:1887:ARG:NH2	1:A:4262:GLN:OE1	2.52	0.42
1:A:2201:GLY:O	1:A:2205:GLU:HG2	2.19	0.42
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.34	0.42
1:A:2777:TYR:HE1	1:A:2794:TYR:HB3	1.84	0.42
1:A:2828:GLU:OE1	1:A:2828:GLU:HA	2.20	0.42
1:A:2948:ARG:HH11	1:A:2948:ARG:HG2	1.84	0.42
1:A:3162:ALA:HA	1:A:3166:GLY:HA2	2.01	0.42
1:A:4096:LEU:HB3	1:A:4099:VAL:HG11	2.01	0.42
1:A:2605:LEU:HD22	1:A:2709:VAL:HG11	2.01	0.42
1:A:3132:LYS:NZ	1:A:3137:PRO:HB3	2.33	0.42
1:A:3491:LYS:HB3	1:A:3491:LYS:HE3	1.77	0.42
1:A:3591:ASP:OD1	1:A:3596:ALA:HB3	2.20	0.42
1:A:3831:PHE:HZ	1:A:3870:ARG:HB3	1.84	0.42
1:A:4629:LYS:HG2	1:A:4630:GLU:OE1	2.20	0.42
1:A:1651:GLN:OE1	1:A:1663:SER:OG	2.29	0.42
1:A:2041:MET:HE2	1:A:2041:MET:HB3	1.83	0.42
1:A:2822:ILE:CG2	1:A:2865:LYS:HD3	2.50	0.42
1:A:3046:SER:O	1:A:3050:LEU:HG	2.19	0.42
1:A:3822:HIS:HE1	1:A:3823:PHE:CZ	2.36	0.42
1:A:1623:ARG:NE	1:A:1637:LEU:HD22	2.35	0.42
1:A:2603:MET:HE1	4:A:4703:ANP:H2'	2.01	0.42
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	2.02	0.42
1:A:4096:LEU:HB3	1:A:4099:VAL:CG1	2.50	0.42
1:A:2590:PRO:HG3	1:A:2687:VAL:HG21	2.01	0.42
1:A:3626:ALA:HB1	1:A:3631:ASN:O	2.19	0.42
1:A:1594:ILE:HG13	1:A:1597:VAL:HB	2.02	0.42
1:A:1998:THR:HG23	1:A:2006:VAL:C	2.45	0.42
1:A:1599:ARG:HH11	1:A:1603:ARG:HE	1.68	0.41
1:A:2613:PRO:HD2	1:A:2614:ASP:H	1.84	0.41
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.19	0.41
1:A:4410:PHE:O	1:A:4414:GLU:OE2	2.37	0.41
1:A:1558:LYS:N	1:A:1558:LYS:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:GLU:OE1	1:A:1620:GLU:HA	2.20	0.41
1:A:1992:LYS:HD2	1:A:1992:LYS:HA	1.67	0.41
1:A:2247:VAL:HG13	1:A:2298:ARG:HH12	1.84	0.41
1:A:3708:LEU:HD22	1:A:3812:TYR:CD2	2.54	0.41
1:A:4446:ASN:N	1:A:4446:ASN:OD1	2.53	0.41
1:A:1571:ILE:HD13	1:A:1607:LEU:HD12	2.03	0.41
1:A:2195:ASP:O	1:A:2198:GLU:HG2	2.21	0.41
1:A:2562:VAL:HG11	1:A:2807:PHE:CD1	2.55	0.41
1:A:2783:ARG:HD3	1:A:2845:TRP:CH2	2.55	0.41
1:A:2872:LEU:HD12	1:A:2920:LEU:HD11	2.01	0.41
1:A:4182:LEU:HD11	1:A:4277:SER:OG	2.21	0.41
1:A:4384:ALA:O	1:A:4388:LEU:HD23	2.21	0.41
1:A:1475:LEU:HD12	1:A:1591:VAL:HG21	2.01	0.41
1:A:1940:ALA:O	1:A:1944:ILE:HG13	2.21	0.41
1:A:2922:ILE:HG12	1:A:2933:LEU:HD21	2.02	0.41
1:A:3614:PHE:HE2	1:A:3641:TYR:HA	1.86	0.41
1:A:3815:MET:HE2	1:A:3832:PHE:HB2	2.01	0.41
1:A:3989:ARG:HB2	1:A:4004:MET:CE	2.50	0.41
1:A:1938:PHE:CE2	1:A:1967:MET:HG2	2.56	0.41
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	2.02	0.41
1:A:2527:PRO:HD3	1:A:2545:TRP:CD1	2.56	0.41
1:A:2974:GLU:HA	1:A:2977:ARG:HH11	1.85	0.41
1:A:2992:PHE:HE2	1:A:3008:MET:HE1	1.86	0.41
1:A:3614:PHE:CE2	1:A:3641:TYR:HA	2.56	0.41
1:A:4431:LEU:HD21	1:A:4464:TRP:HH2	1.86	0.41
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	2.02	0.41
1:A:1591:VAL:O	1:A:1594:ILE:HG12	2.20	0.41
1:A:2461:MET:CE	1:A:2497:ALA:HA	2.51	0.41
1:A:2924:ARG:O	1:A:2927:ARG:HG2	2.21	0.41
1:A:3123:PRO:HG2	1:A:3126:MET:HE1	2.03	0.41
1:A:4201:TRP:O	1:A:4202:SER:OG	2.38	0.41
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.88	0.41
1:A:1579:MET:HA	1:A:1582:VAL:HG12	2.03	0.41
1:A:2137:LEU:O	1:A:2141:VAL:HG23	2.21	0.41
1:A:2495:VAL:O	1:A:2499:LEU:HD23	2.21	0.41
1:A:2728:LEU:HD23	1:A:2728:LEU:HA	1.92	0.41
1:A:3636:GLN:HA	1:A:3680:SER:O	2.19	0.41
1:A:3909:LEU:C	1:A:4344:LEU:HD21	2.46	0.41
1:A:4185:TRP:HD1	1:A:4272:LEU:HD11	1.85	0.41
1:A:1508:LYS:HG2	1:A:1513:TYR:CE1	2.56	0.41
1:A:2073:PHE:HZ	1:A:2096:VAL:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2347:ASP:OD2	1:A:2348:LEU:N	2.53	0.41
1:A:2995:ASP:CG	1:A:2996:GLU:H	2.29	0.41
1:A:3923:ARG:HG2	1:A:3924:ILE:N	2.35	0.41
1:A:1498:LYS:HA	1:A:1501:ILE:HG12	2.02	0.41
1:A:1539:ASP:O	1:A:1543:ARG:HG2	2.21	0.41
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	2.01	0.41
1:A:2175:MET:HE2	1:A:2175:MET:HB3	1.81	0.41
1:A:2320:ASP:OD1	1:A:2358:ARG:NH1	2.54	0.41
1:A:2679:VAL:O	1:A:2683:ILE:HG13	2.21	0.41
1:A:2920:LEU:HD23	1:A:2920:LEU:HA	1.94	0.41
1:A:3513:PHE:HZ	1:A:3575:GLU:HB3	1.86	0.41
1:A:3549:ARG:H	1:A:3549:ARG:HG2	1.56	0.41
1:A:3892:LEU:HD12	1:A:3892:LEU:HA	1.81	0.41
1:A:3957:PHE:CE2	1:A:3961:LEU:HD21	2.55	0.41
1:A:4027:LEU:H	1:A:4027:LEU:HD23	1.86	0.41
1:A:2230:LYS:HE3	1:A:2345:VAL:O	2.21	0.41
1:A:2285:ARG:HG3	1:A:2285:ARG:NH1	2.36	0.41
1:A:2484:GLU:O	1:A:2488:ARG:HG3	2.21	0.41
1:A:3923:ARG:HD2	1:A:3927:LEU:HG	2.02	0.41
1:A:4448:LEU:O	1:A:4452:ILE:HG12	2.21	0.41
1:A:1587:LEU:O	1:A:1591:VAL:HG23	2.21	0.40
1:A:3141:GLU:H	1:A:3141:GLU:HG3	1.67	0.40
1:A:3474:ARG:NH2	1:A:3764:ASP:N	2.67	0.40
1:A:3566:SER:OG	1:A:3602:ASN:ND2	2.50	0.40
1:A:3639:GLU:OE2	1:A:3681:THR:OG1	2.39	0.40
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.82	0.40
1:A:4248:ALA:O	1:A:4262:GLN:NE2	2.48	0.40
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.56	0.40
1:A:4401:THR:HG22	1:A:4403:GLU:HG3	2.03	0.40
1:A:1912:LYS:NZ	2:A:4701:ADP:O2B	2.53	0.40
1:A:2797:ARG:O	1:A:2800:THR:HG22	2.22	0.40
1:A:3881:ILE:HD13	1:A:4006:HIS:ND1	2.36	0.40
1:A:4379:THR:HA	1:A:4382:THR:HG22	2.02	0.40
1:A:4527:TYR:HD2	1:A:4558:PHE:HZ	1.70	0.40
1:A:1556:ASP:OD2	1:A:1644:SER:OG	2.36	0.40
1:A:1557:ILE:HG23	1:A:1558:LYS:HD3	2.02	0.40
1:A:1565:THR:O	1:A:1569:GLN:HG3	2.21	0.40
1:A:2759:ILE:HG13	1:A:2759:ILE:O	2.21	0.40
1:A:2819:GLU:HA	1:A:2865:LYS:NZ	2.37	0.40
1:A:2890:ARG:HG2	1:A:2894:LYS:HE3	2.02	0.40
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4178:ARG:NH1	1:A:4296:MET:HE2	2.36	0.40
1:A:4445:THR:HG23	1:A:4448:LEU:H	1.86	0.40
1:A:2464:GLN:CB	1:A:2583:THR:HG23	2.51	0.40
1:A:2471:GLN:OE1	1:A:2471:GLN:HA	2.22	0.40
1:A:3128:VAL:HG11	1:A:3148:VAL:HG13	2.04	0.40
1:A:3215:VAL:HG21	1:A:3478:LEU:HD23	2.04	0.40
1:A:3485:GLU:O	1:A:3489:TRP:CD1	2.75	0.40
1:A:1506:ALA:HB1	1:A:3667:GLN:NE2	2.36	0.40
1:A:2016:ILE:HD12	1:A:2036:PHE:CZ	2.57	0.40
1:A:2561:LYS:O	1:A:2567:VAL:HG21	2.21	0.40
1:A:2823:ARG:NH2	1:A:2871:ILE:HA	2.37	0.40
1:A:2914:GLU:O	1:A:2918:HIS:HD2	2.03	0.40
1:A:3779:GLU:HG2	1:A:3782:ARG:HH12	1.85	0.40
1:A:4495:ALA:HB1	1:A:4503:GLU:OE1	2.22	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	2844/4646 (61%)	2751 (97%)	92 (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	2544/4125 (62%)	2538 (100%)	6 (0%)	92 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2572	LEU
1	A	2901	TYR
1	A	2904	GLU
1	A	3540	ASN
1	A	3978	THR
1	A	4391	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1748	GLN
1	A	1881	GLN
1	A	1979	GLN
1	A	1985	HIS
1	A	2003	ASN
1	A	2067	ASN
1	A	2139	GLN
1	A	2263	HIS
1	A	2414	GLN
1	A	2476	HIS
1	A	2685	GLN
1	A	2789	GLN
1	A	2827	HIS
1	A	3087	ASN
1	A	3104	GLN
1	A	3185	ASN
1	A	3188	HIS
1	A	3538	GLN
1	A	3584	ASN
1	A	3667	GLN
1	A	3799	GLN
1	A	3822	HIS
1	A	3956	GLN

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Mol	Chain	Res	Type
1	A	4029	HIS
1	A	4117	GLN
1	A	4404	ASN
1	A	4526	GLN
1	A	4566	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)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ANP	A	4703	5	29,33,33	1.14	4 (13%)	31,52,52	0.91	1 (3%)
2	ADP	A	4704	-	24,29,29	0.87	0	29,45,45	1.22	2 (6%)
2	ADP	A	4701	5	24,29,29	0.87	0	29,45,45	1.23	2 (6%)
3	ATP	A	4702	5	28,33,33	0.66	0	34,52,52	0.60	1 (2%)

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
4	ANP	A	4703	5	-	3/14/38/38	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4701	5	-	2/12/32/32	0/3/3/3
3	ATP	A	4702	5	-	7/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4703	ANP	PB-O3A	-2.53	1.55	1.59
4	A	4703	ANP	PG-O1G	2.49	1.49	1.46
4	A	4703	ANP	PG-N3B	2.38	1.69	1.63
4	A	4703	ANP	PB-O1B	2.24	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	ADP	N3-C2-N1	-3.73	123.61	128.67
2	A	4704	ADP	N3-C2-N1	-3.65	123.71	128.67
2	A	4701	ADP	C4-C5-N7	-2.73	106.45	109.34
2	A	4704	ADP	C4-C5-N7	-2.59	106.60	109.34
4	A	4703	ANP	C5-C6-N6	2.35	123.89	120.31
3	A	4702	ATP	C5-C6-N6	2.34	123.87	120.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	PB-O3B-PG-O3G
3	A	4702	ATP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O3A
4	A	4703	ANP	PB-N3B-PG-O1G
4	A	4703	ANP	PG-N3B-PB-O1B
4	A	4703	ANP	PG-N3B-PB-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
2	A	4701	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	PG-O3B-PB-O2B
3	A	4702	ATP	PA-O3A-PB-O2B

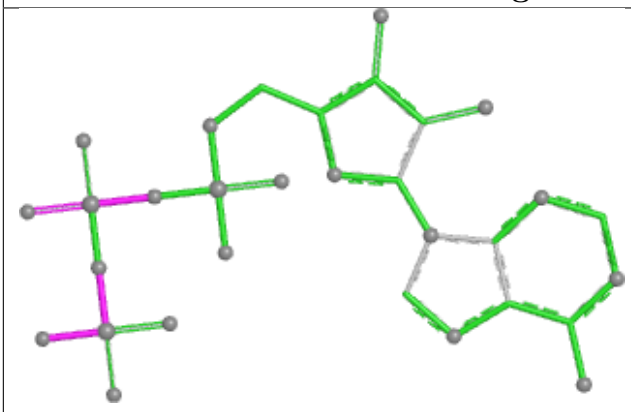
There are no ring outliers.

4 monomers are involved in 11 short contacts:

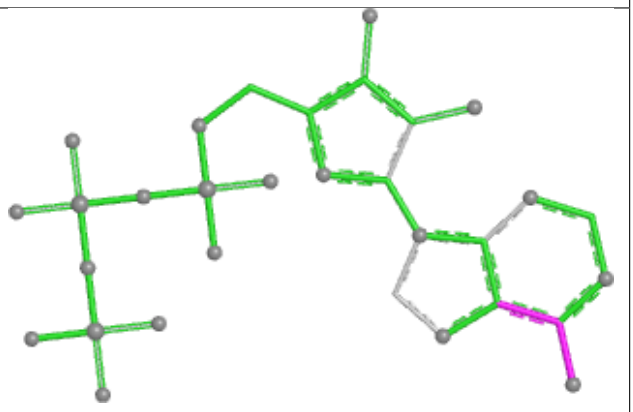
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	4	0
2	A	4704	ADP	1	0
2	A	4701	ADP	4	0
3	A	4702	ATP	2	0

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.

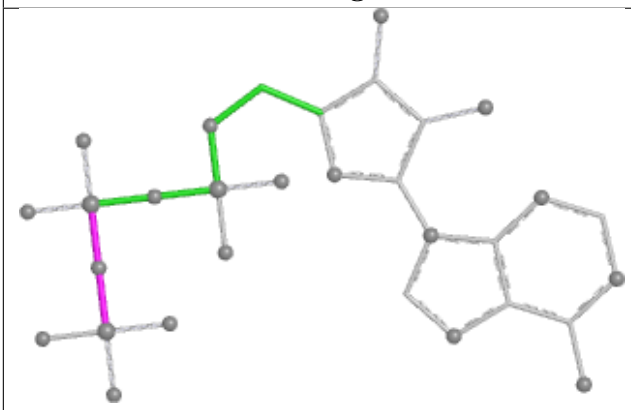
Ligand ANP A 4703



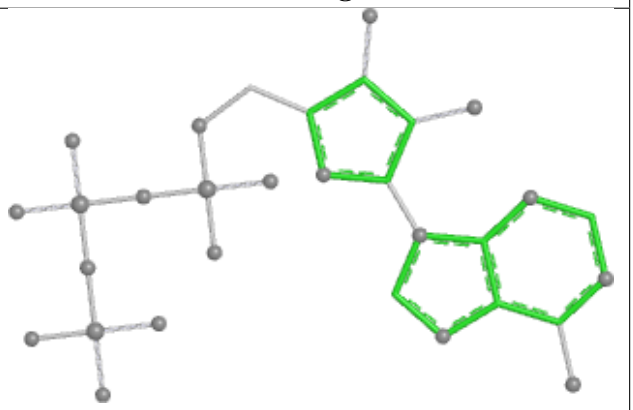
Bond lengths



Bond angles

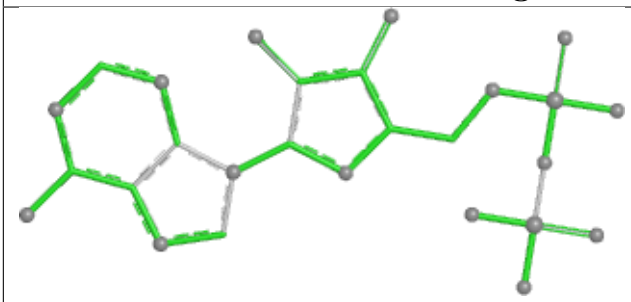


Torsions

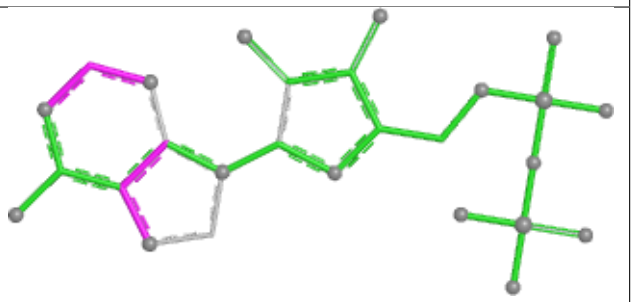


Rings

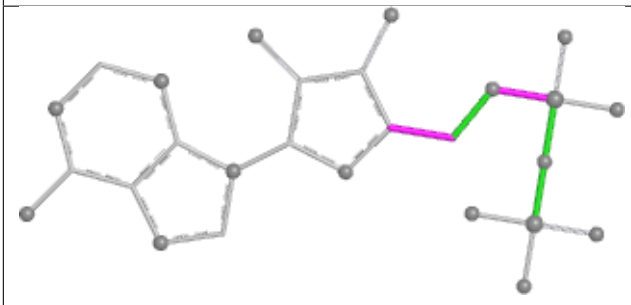
Ligand ADP A 4704



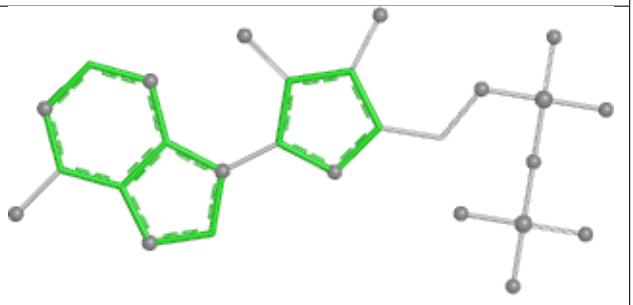
Bond lengths



Bond angles

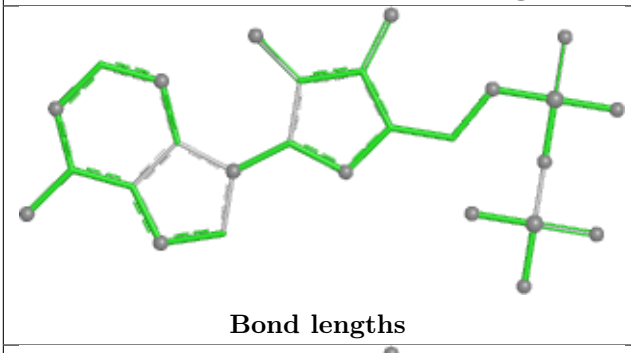


Torsions

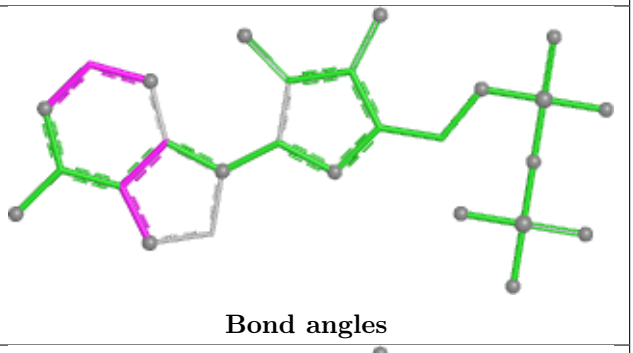


Rings

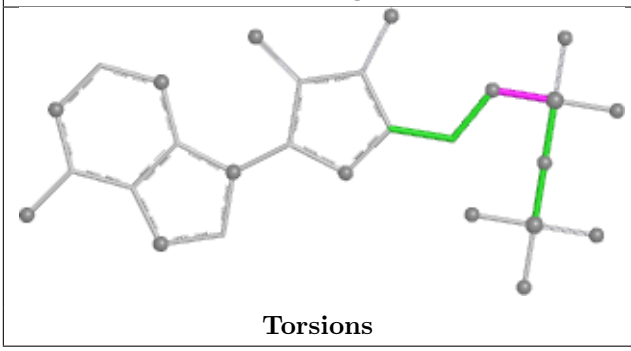
Ligand ADP A 4701



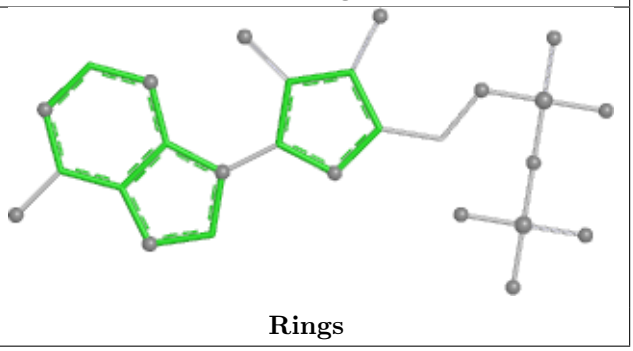
Bond lengths



Bond angles

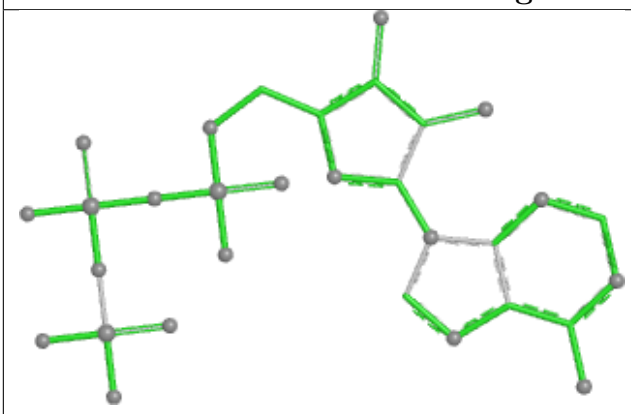


Torsions

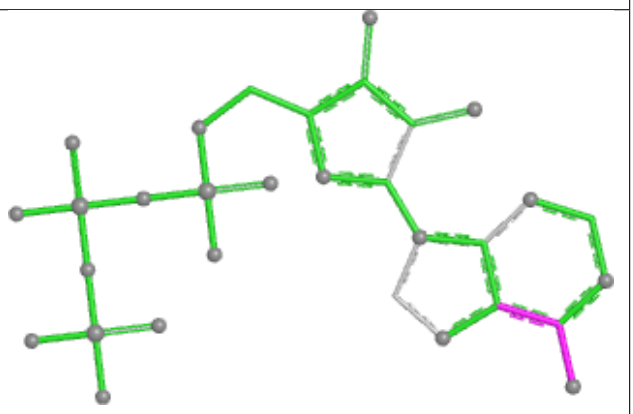


Rings

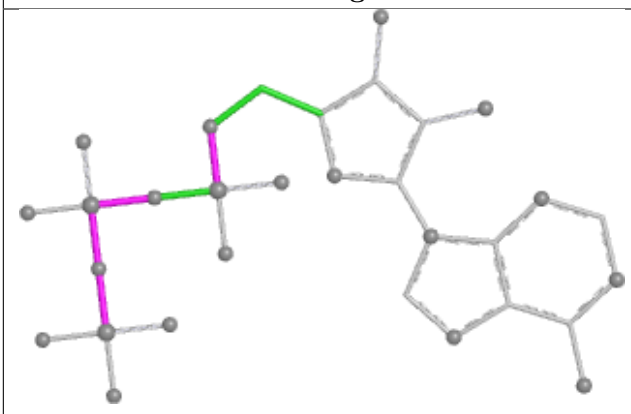
Ligand ATP A 4702



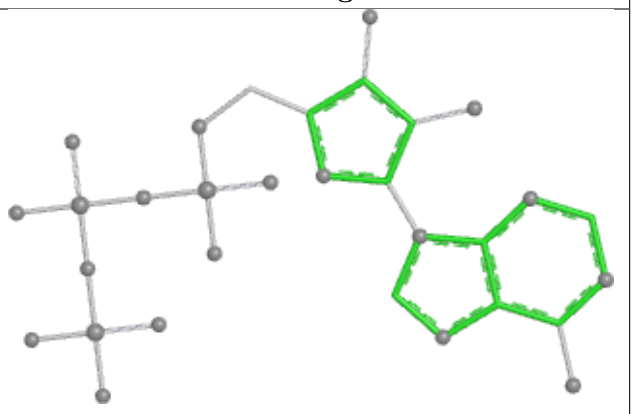
Bond lengths



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.

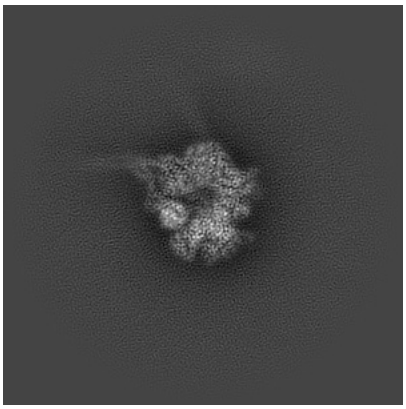
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46860. These allow visual inspection of the internal detail of the map and identification of artifacts.

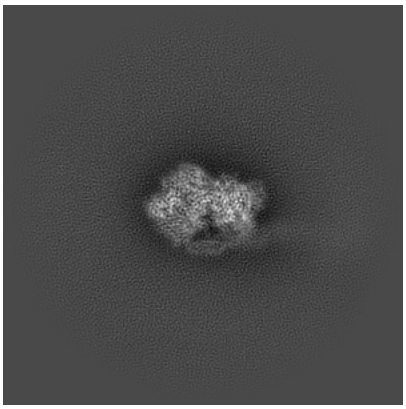
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

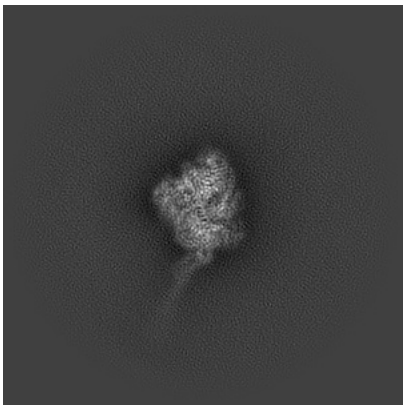
6.1.1 Primary map



X

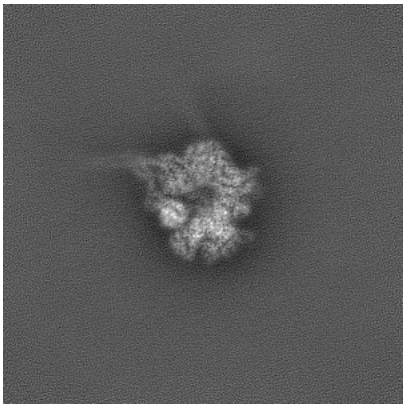


Y

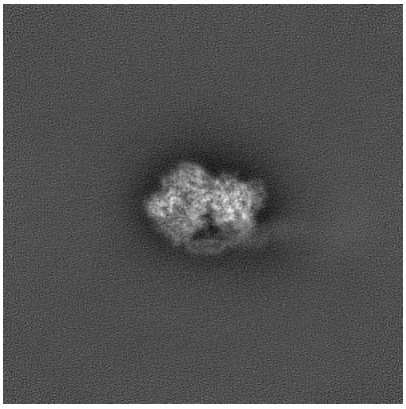


Z

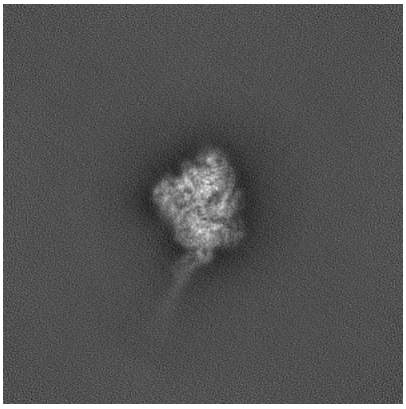
6.1.2 Raw map



X



Y

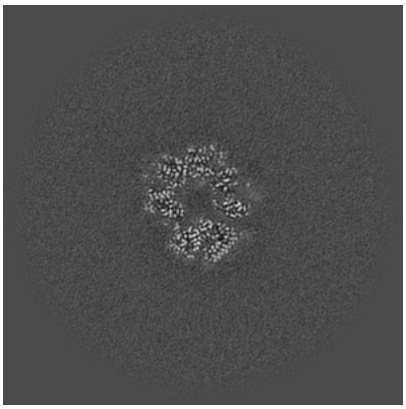


Z

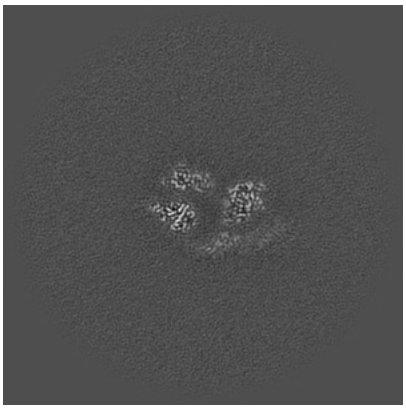
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

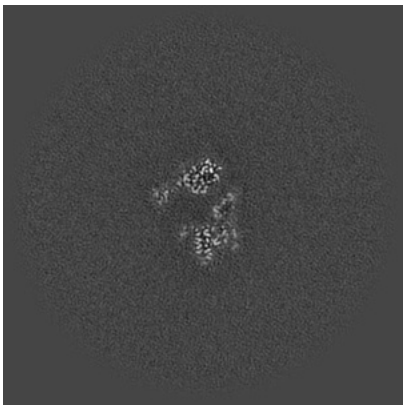
6.2.1 Primary map



X Index: 192

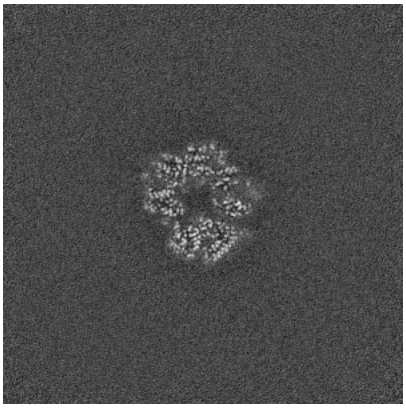


Y Index: 192

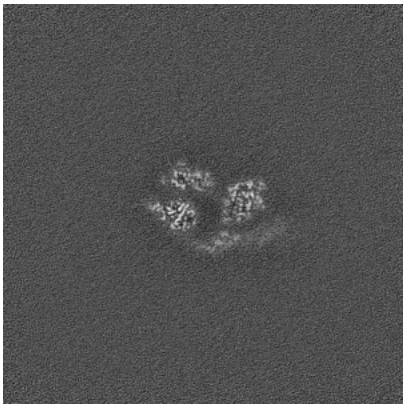


Z Index: 192

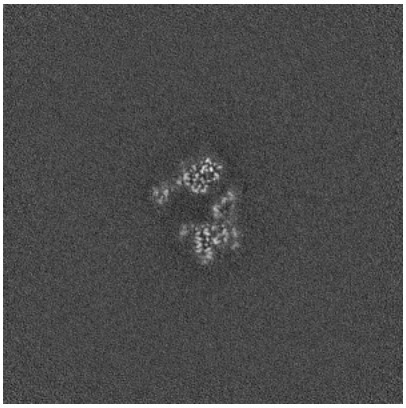
6.2.2 Raw map



X Index: 192



Y Index: 192

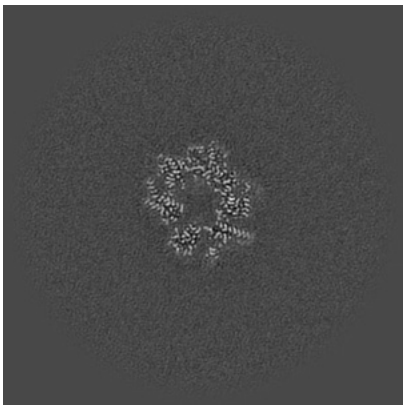


Z Index: 192

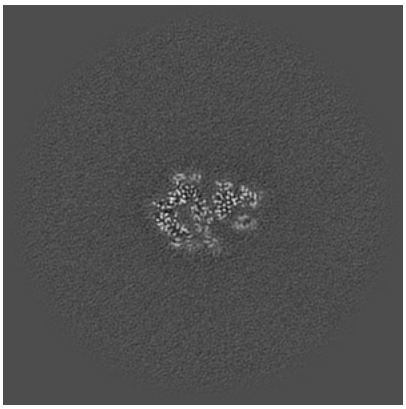
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

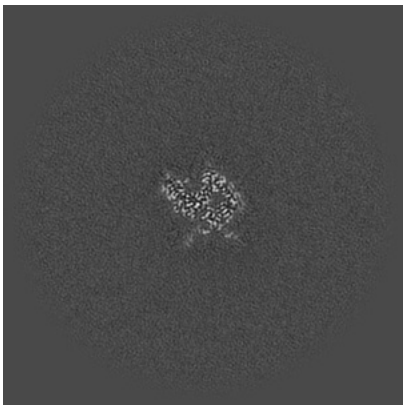
6.3.1 Primary map



X Index: 196

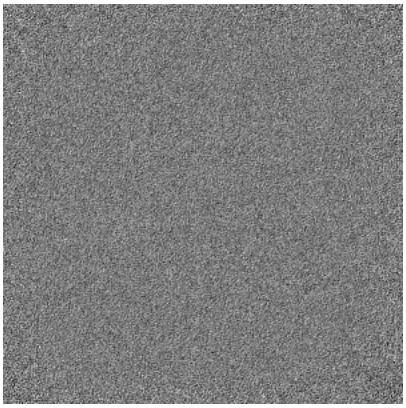


Y Index: 209

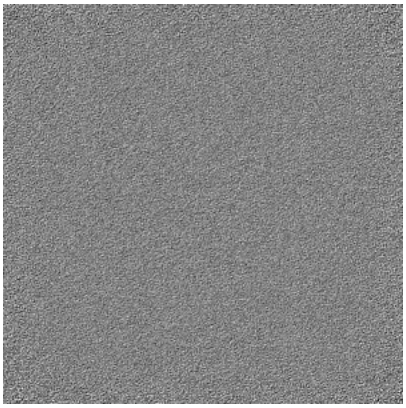


Z Index: 169

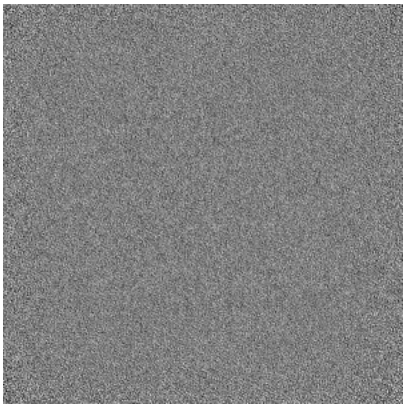
6.3.2 Raw map



X Index: 0



Y Index: 0

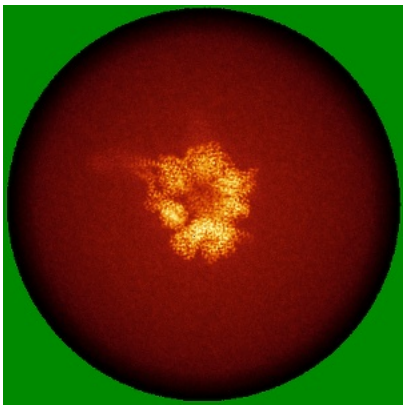


Z Index: 0

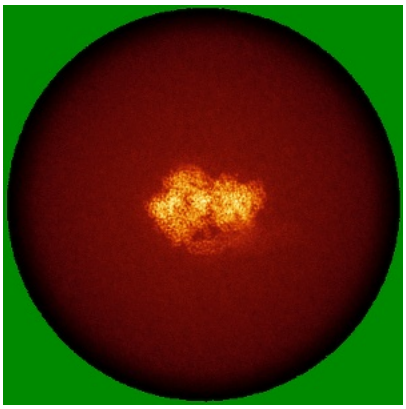
The images above show the largest variance slices of the map in three orthogonal directions.

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

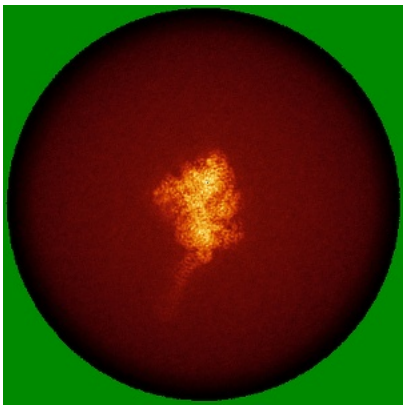
6.4.1 Primary map



X

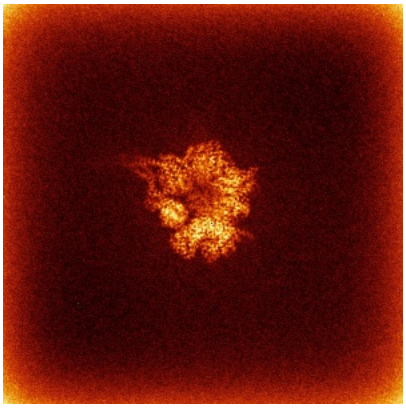


Y

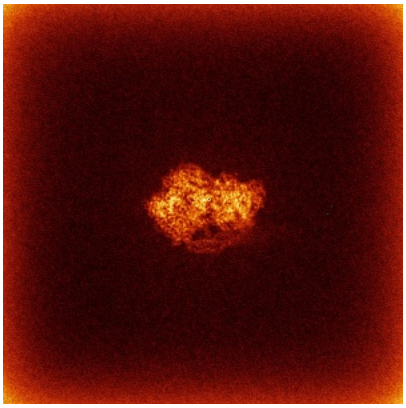


Z

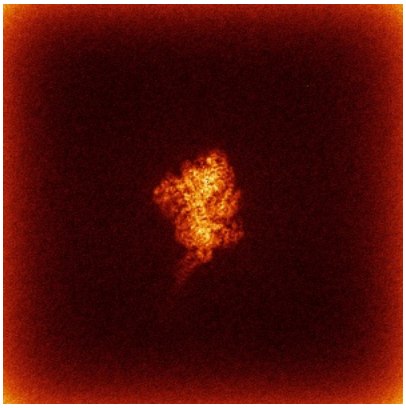
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

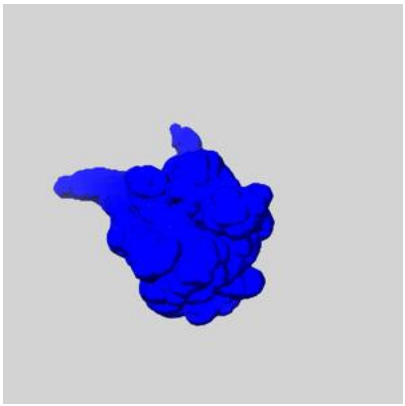
6.6 Mask visualisation

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

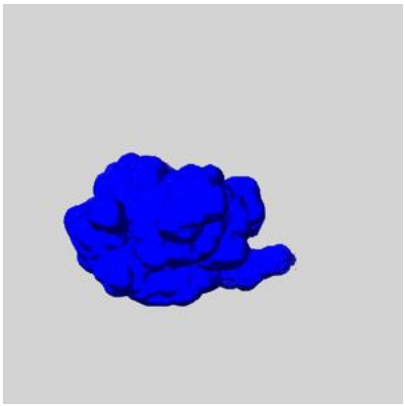
A mask typically either:

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

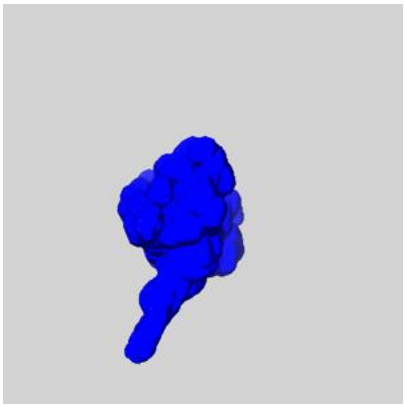
6.6.1 emd_46860_msk_1.map



X



Y

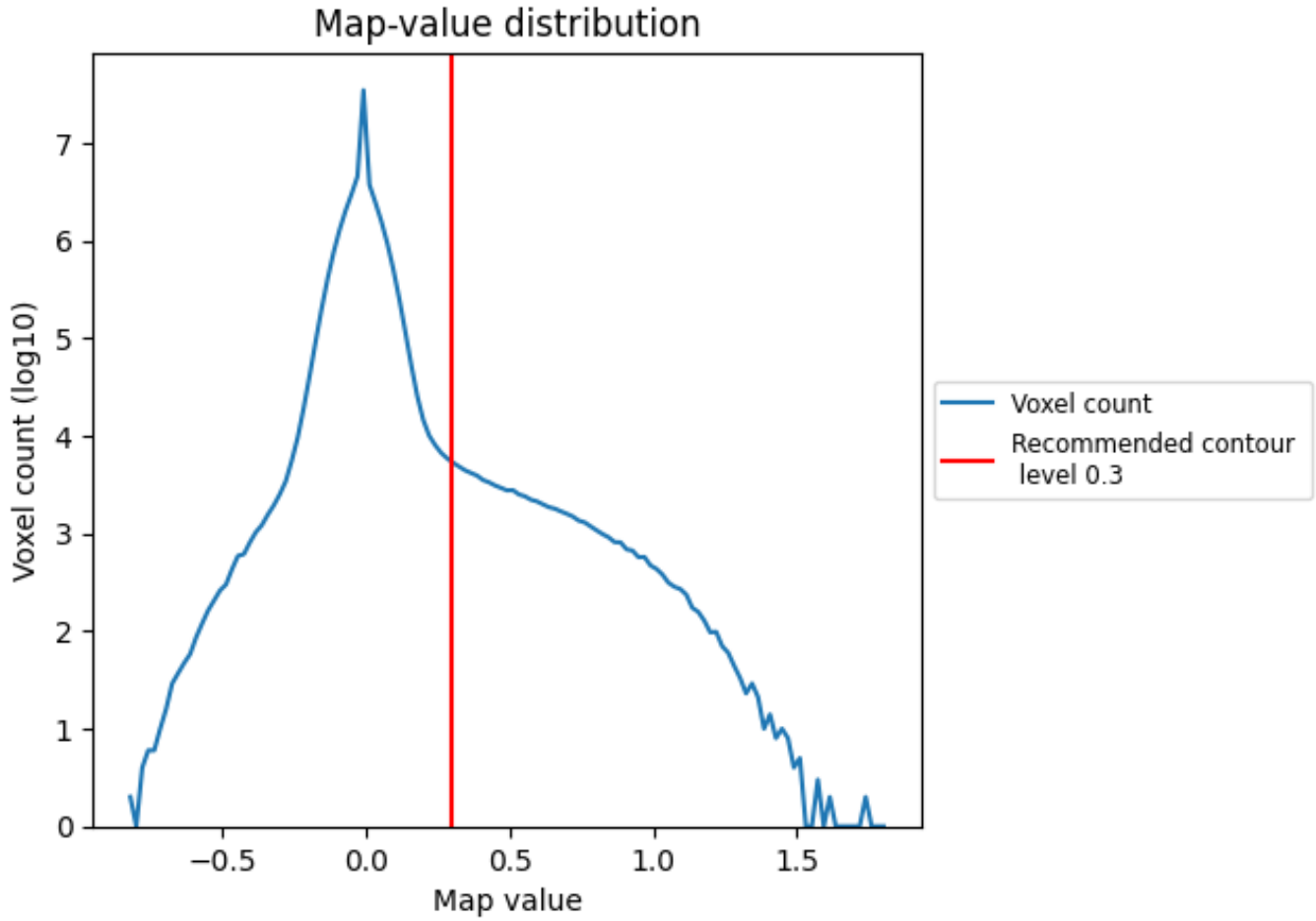


Z

7 Map analysis

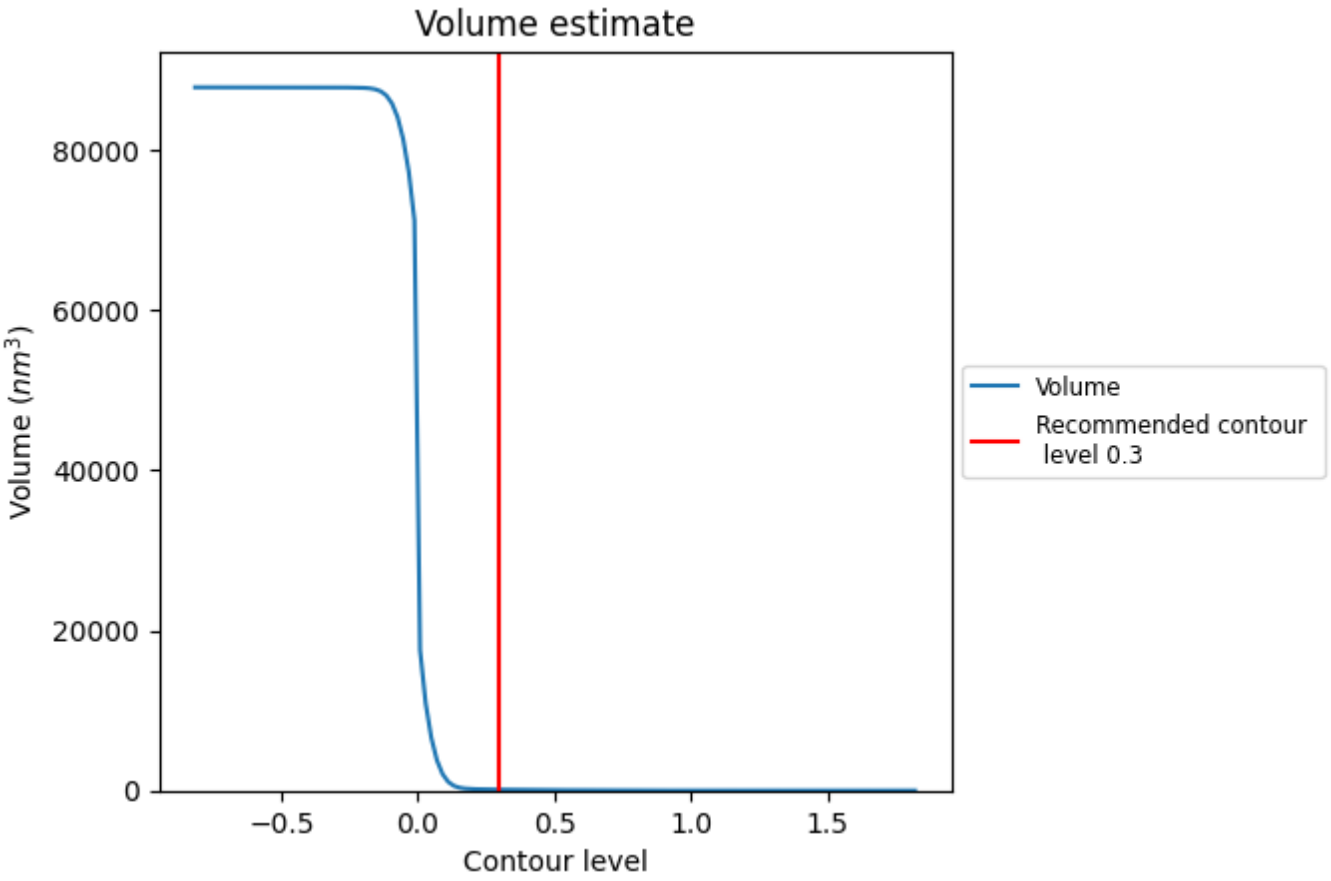
This section contains the results of statistical analysis of the map.

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.

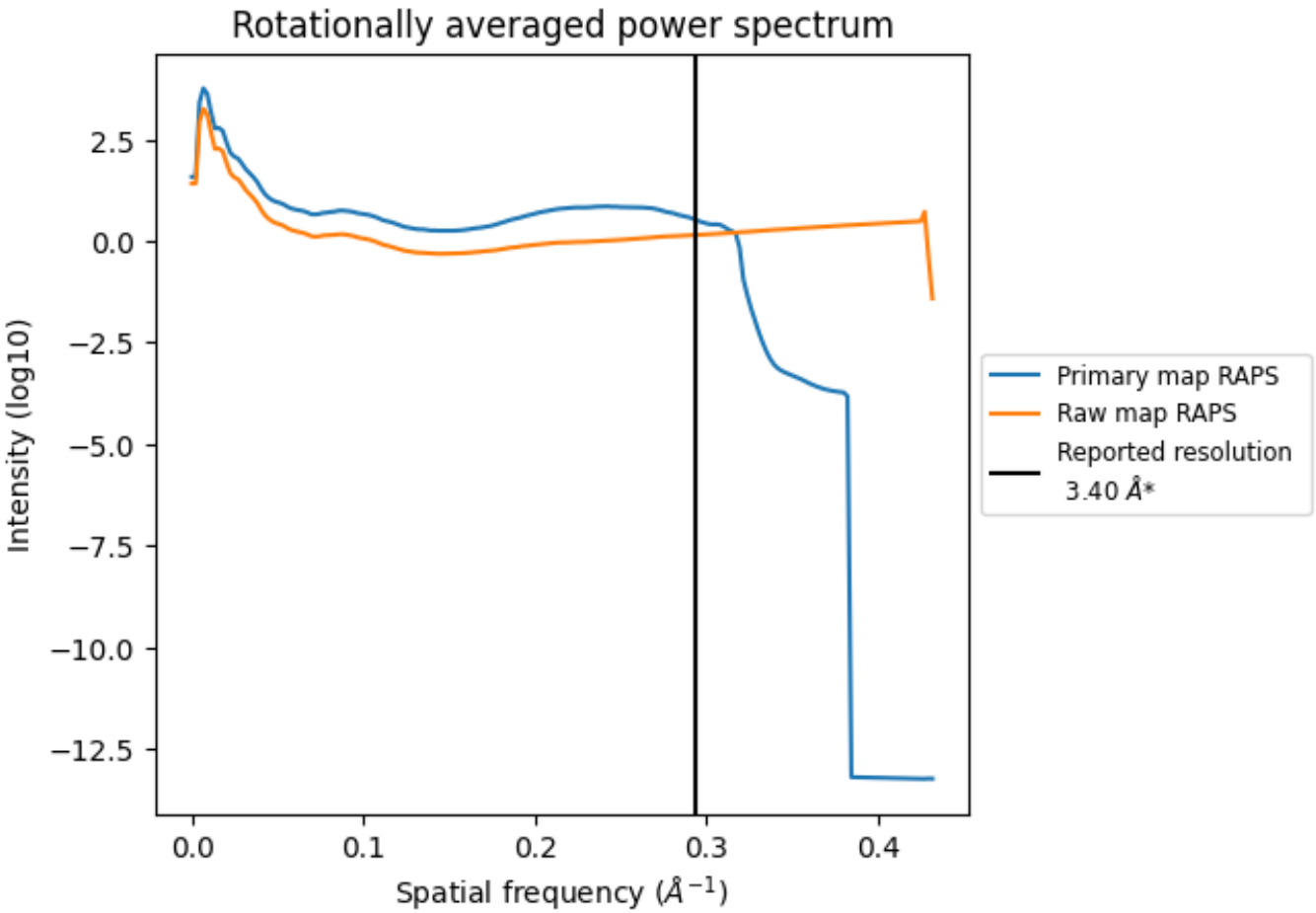
7.2 Volume estimate



The volume at the recommended contour level is 118 nm^3; this corresponds to an approximate mass of 107 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)

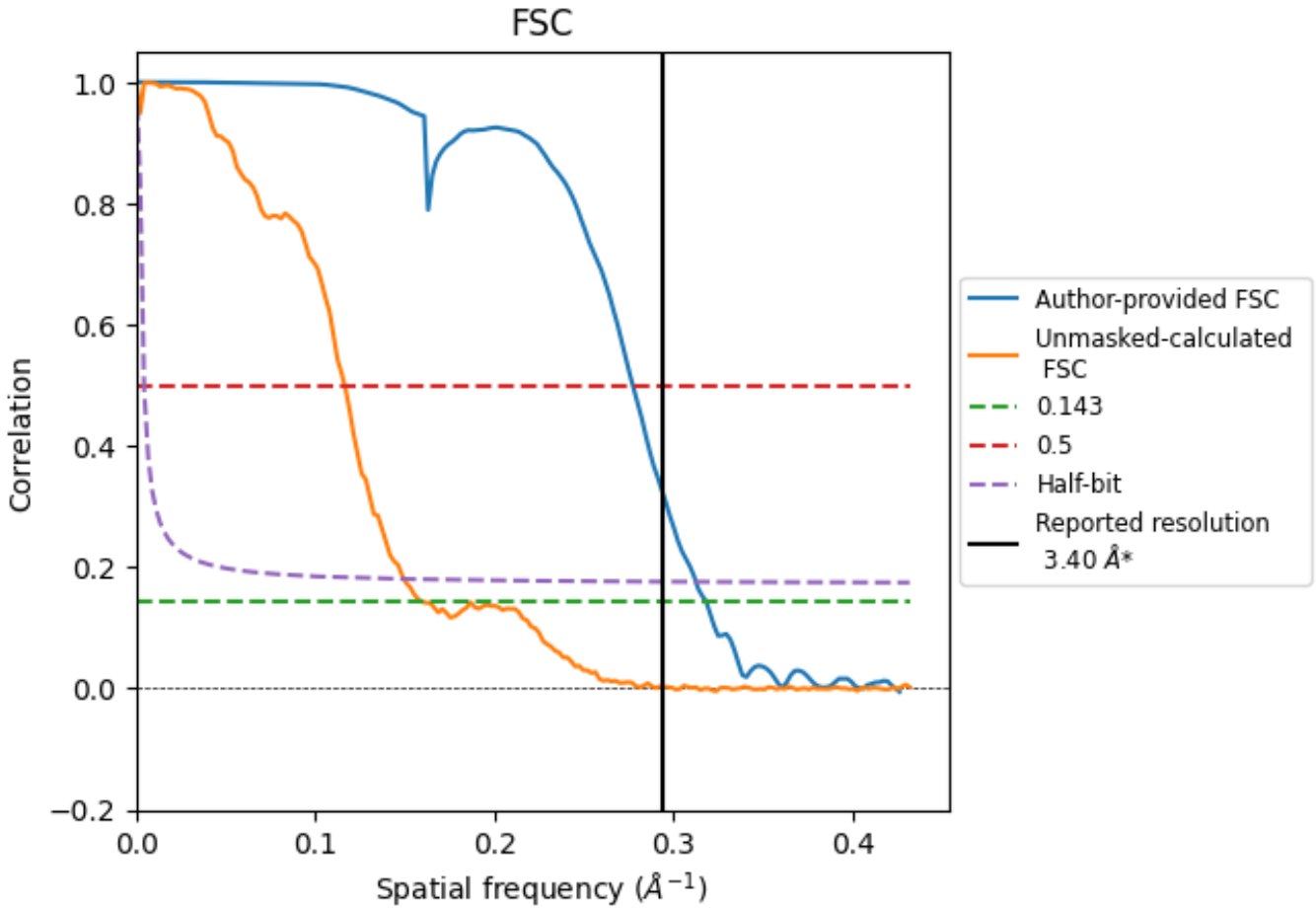


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

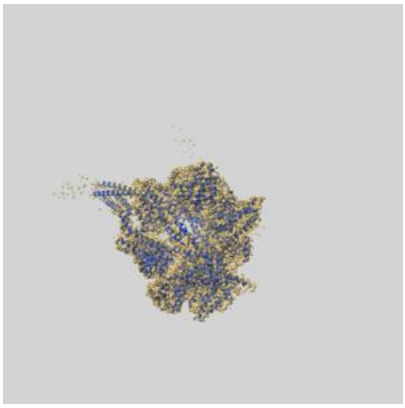
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.14	3.60	3.20
Unmasked-calculated*	6.27	8.58	6.68

*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 6.27 differs from the reported value 3.4 by more than 10 %

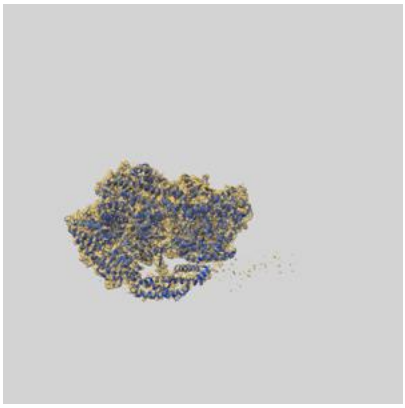
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46860 and PDB model 9DH9. Per-residue inclusion information can be found in section 3 on page 6.

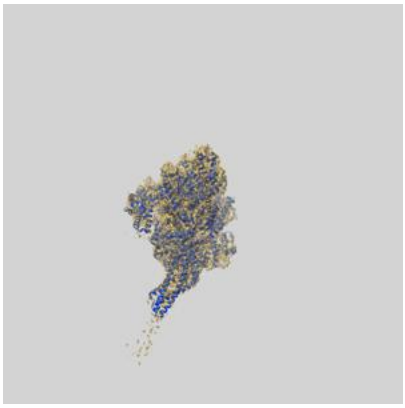
9.1 Map-model overlay



X



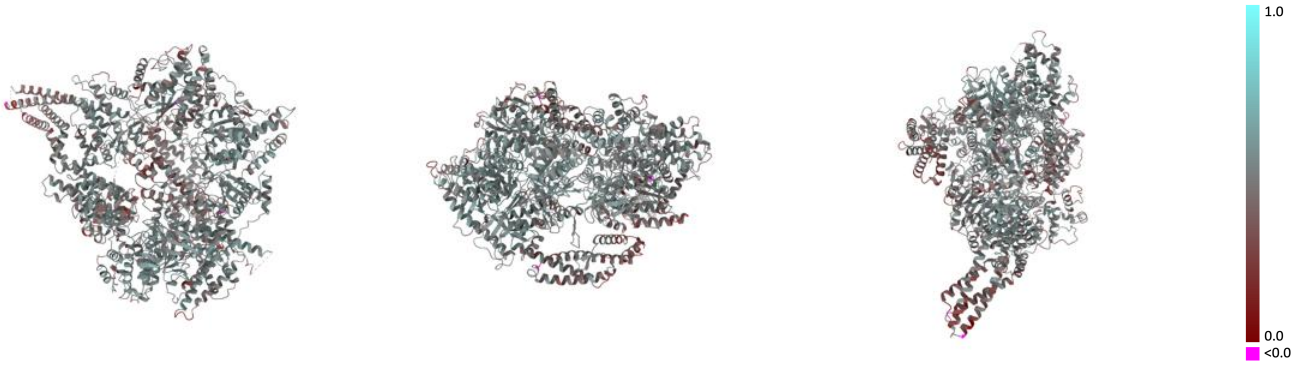
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

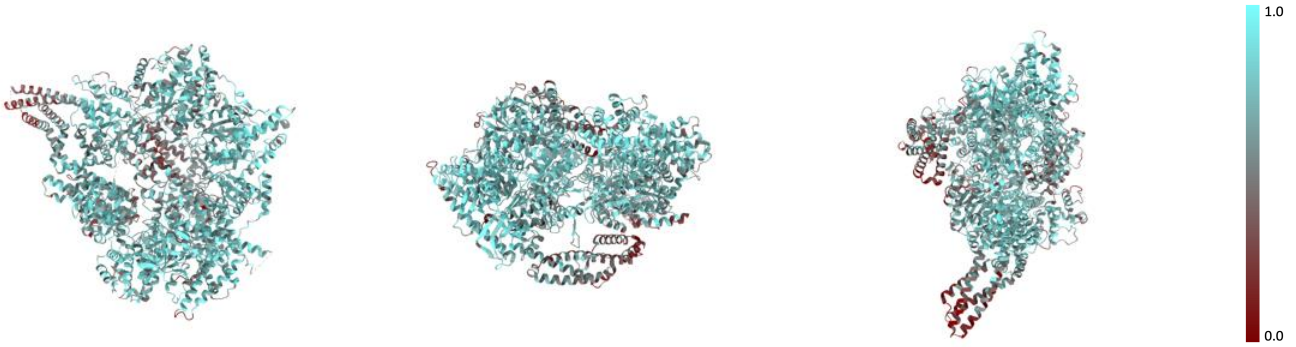
9.2 Q-score mapped to coordinate model



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.

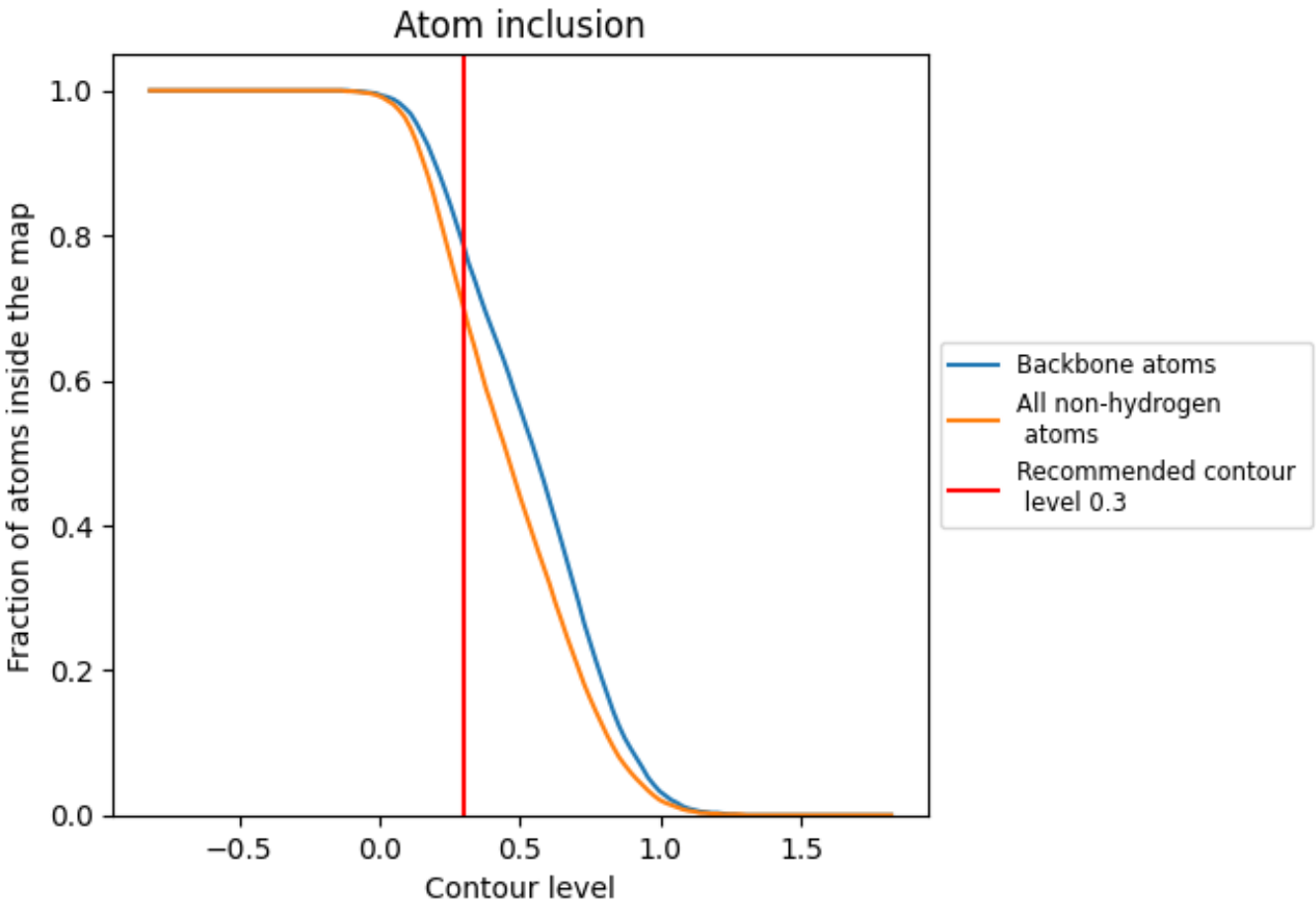
9.3 Atom inclusion mapped to coordinate model



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7000	0.4880
A	0.7000	0.4880