wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 05:11 am GMT

PDB ID	:	6ZYY
EMDB ID	:	EMD-11581
Title	:	Outer Dynein Arm-Shulin complex - Dyh3 motor region (Tetrahymena thermophila)
Authors	:	Mali, G.R.; Abid Ali, F.; Lau, C.K.; Begum, F.; Boulanger, J.; Howe, J.D.; Chen, Z.A.; Rappsilber, J.; Skehel, M.; Carter, A.P.
Deposited on	:	2020-08-03
Resolution	:	4.40 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

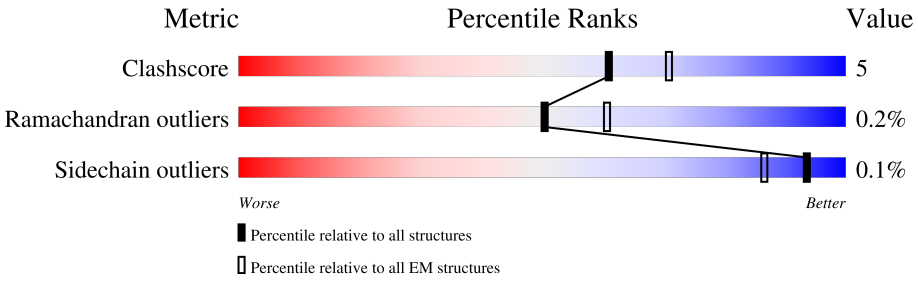
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

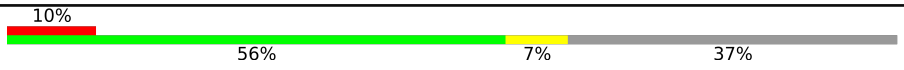
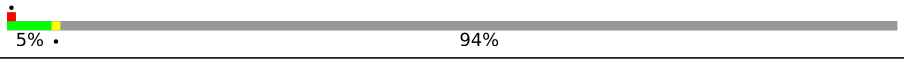
The reported resolution of this entry is 4.40 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	4620	
2	Y	1200	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22453 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.

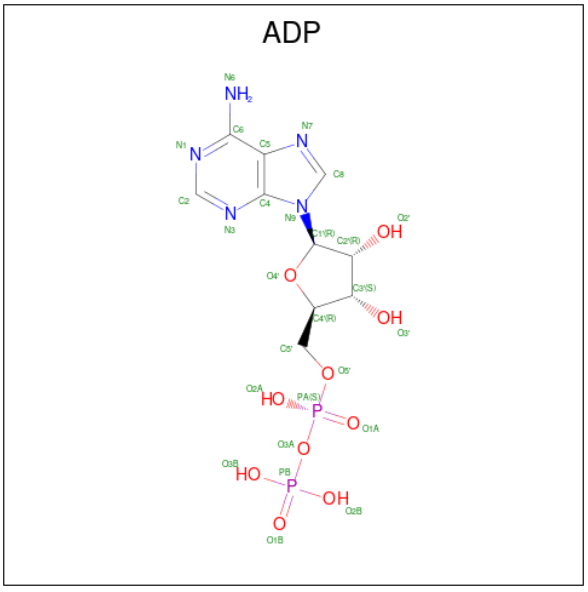
- Molecule 1 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	2901	21875	13931	3736	4092	116	0	0

- Molecule 2 is a protein called Shulin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	Y	66	466	303	89	74	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	C	1	81	30	15	30	6	0
3	C	1	Total	C	N	O	P	0
			81	30	15	30	6	

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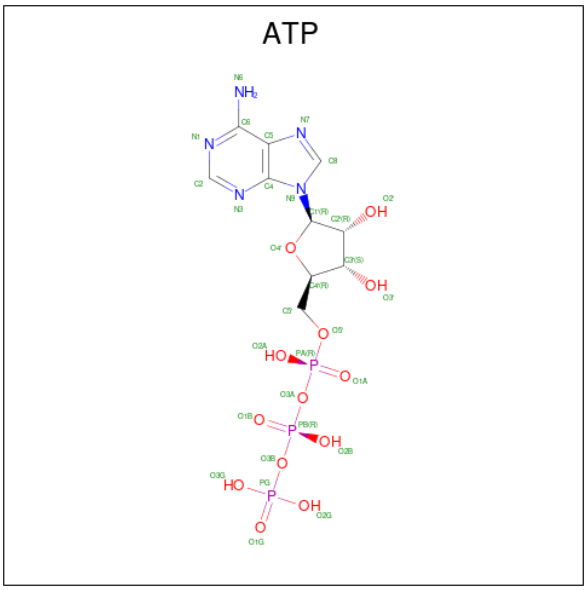
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			81	30	15	30	6	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



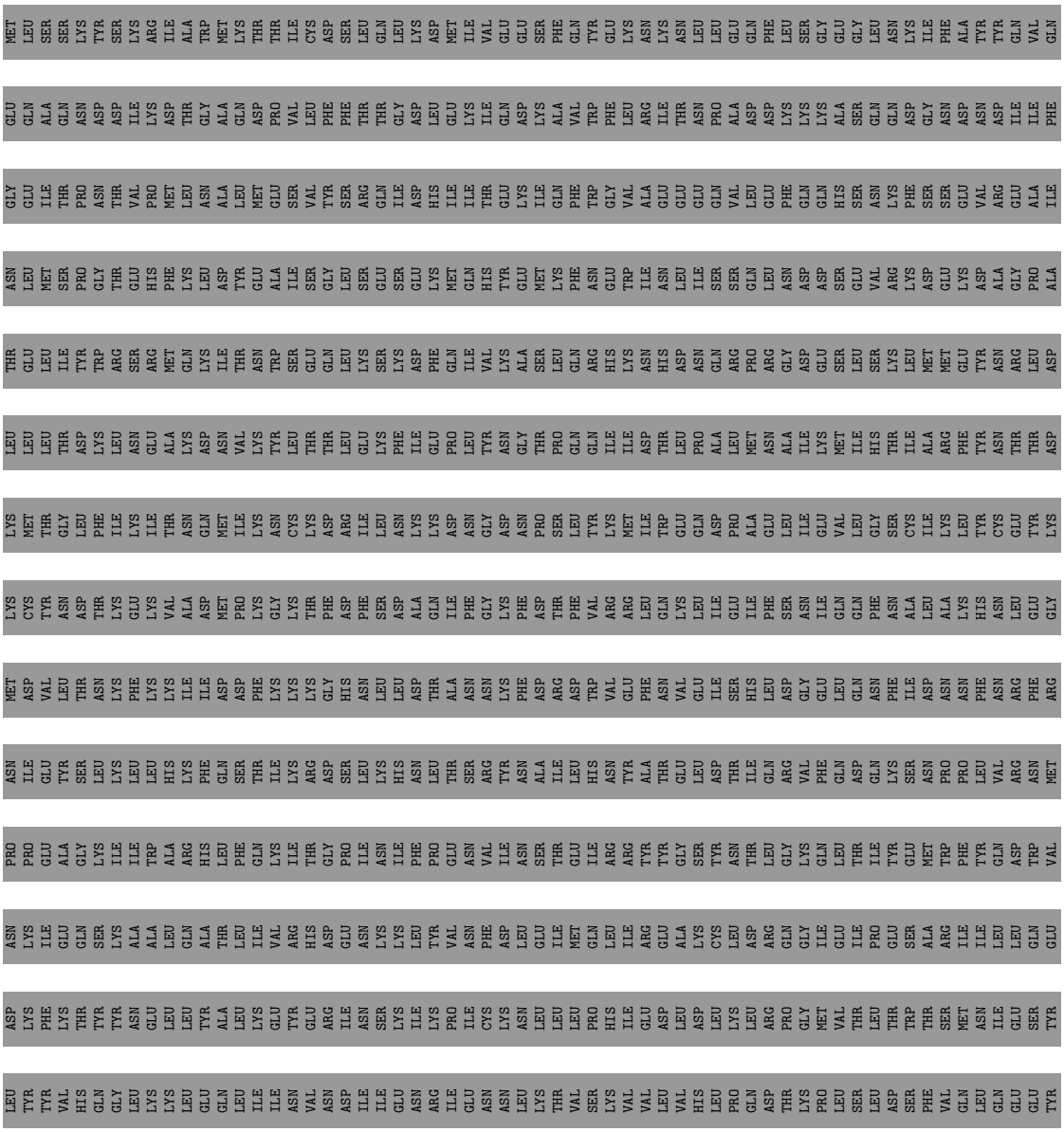
Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

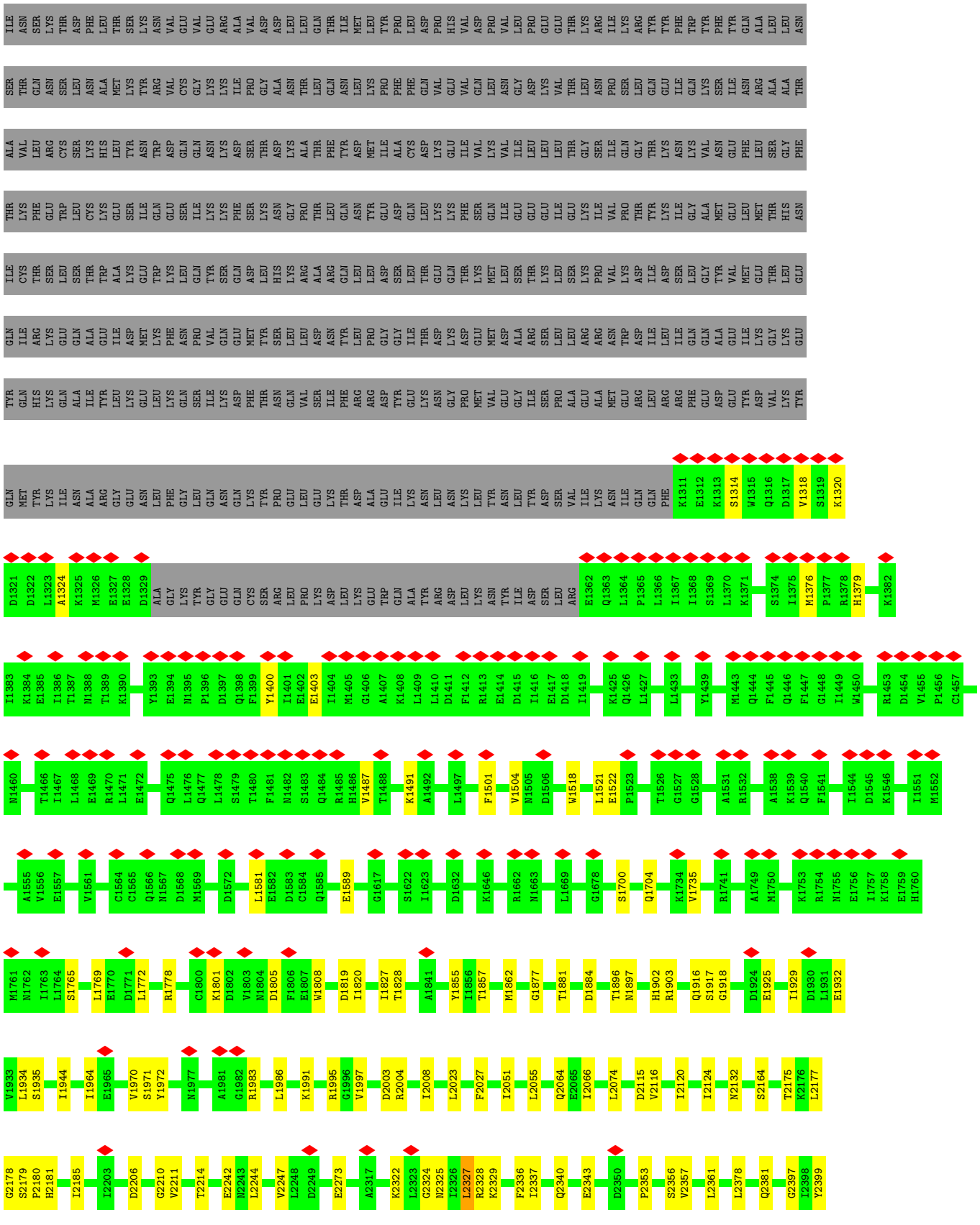
3 Residue-property plots (i)

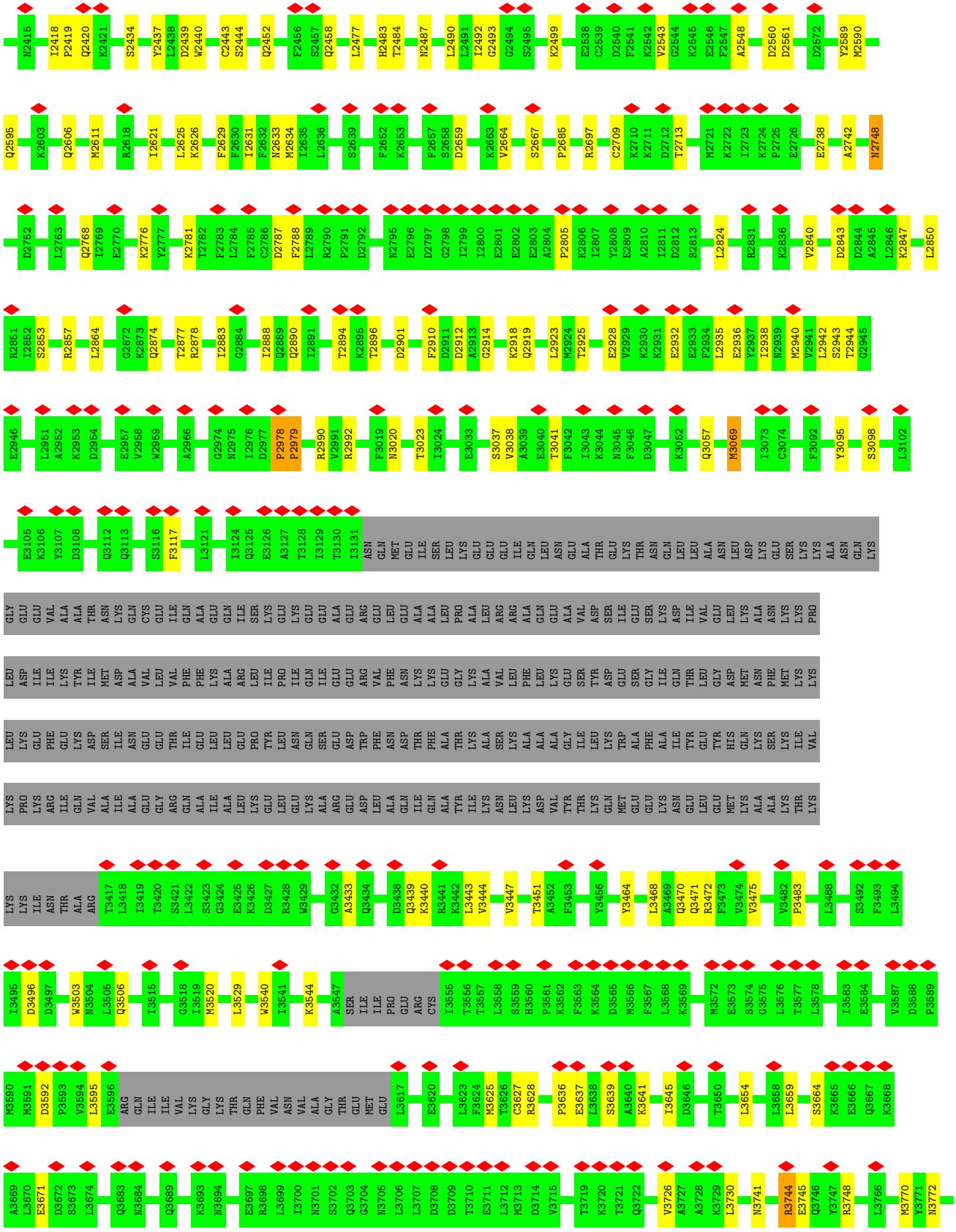
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain C:




ILE ASN SER LYS THR ASP PHE LEU THR SER LYS ASN VAL GLU VAL GLU GLU ARG ALA VAL ASP ASP LEU LEU GLN THR ILE MET LEU TYR PRO LEU ASP PRO HIS VAL ASP PRO VAL LEU PRO GLU GLU THR LYS ARG ILE LYS ARG TYR TYR PHE TRP TYR PHE TYR GLN ALA LEU LEU ASN
SER THR GLN ASN SER LEU ASN ALA MET LYS TYR ARG VAL CYS GLY LYS LYS ILE PRO GLY ALA ASN THR LEU GLN ASN ALA LEU LYS PRO PHE PHE GLN VAL GLU VAL GLN LEU ASN ASP GLY ASP LYS VAL THR LEU ASN PRO SER LEU GLN GLY THR LYS ASN LEU GLU GLN ILE GLN LYS SER ILE ASN ARG ALA ALA THR
ALA VAL LEU ARG CYS SER LYS HIS LEU TYR ASN TRP ASP GLN GLN ASN LYS ASP SER THR ASP LYS ALA THR PHE TYR ASP MET ILE ALA CYS ASP LYS GLU VAL GLN ILE VAL LYS VAL ILE LEU LEU LEU LEU THR GLY SER ILE GLN GLY THR LYS ASN GLU VAL ASN GLU PHE LEU SER HIS PHE
THR LYS PHE GLU TRP LEU SER CYS LYS GLU SER ILE GLN GLU SER ILE LYS LYS PHE SER LYS ASN GLY PRO THR LEU GLN ASN TYR GLU ASP GLN LEU LYS LYS PHE SER GLN ILE GLU GLU GLU ILE GLU LYS ILE VAL THR GLY ASP TYR TYR LYS ILE GLY ALA MET LEU GLU THR HIS ASN
ILE CYS THR SER LEU SER THR TRP ALA LYS GLU TRP LYS LEU GLN TYR SER GLN ASP LEU HIS LYS ARG ALA ARG GLN LEU LEU ASP SER LEU THR LEU GLU LEU SER LYS PRO VAL LYS ASP ILE ASP SER LEU THR LYS LEU SER LYS ILE GLN LEU GLY TYR VAL MET GLU THR LEU GLU
GLN ILE ARG LYS GLU GLN ILE ASP MET LYS PHE ASN PRO VAL GLN GLU MET TYR SER LEU LEU ASP ASN TYR LEU PRO GLY GLY ILE THR ASP LYS ASP GLU MET ASP ALA ARG SER LEU LEU ARG ARG ASN TRP ASP ILE LEU ILE GLN GLN ALA GLU ILE LYS GLY LYS GLU
TYR GLN HIS LYS GLN ALA ILE TYR LEU LYS GLU LEU LYS GLN SER ILE LYS ASP PHE THR ASN GLN VAL SER ILE PHE ARG ARG ASP TYR GLU LYS ASN GLY TYR LEU VAL GLU GLY ILE SER PRO ALA GLU ALA MET GLU ARG LEU ARG ARG PHE GLU ASP GLU TYR ASP VAL LYS TYR
GLN MET TYR LYS ILE ASN ALA ARG GLY GLU ASN LEU PHE GLY LEU GLN LEU GLU LEU LYS THR ASP ALA GLU ILE LYS ASN LEU ASN LYS LEU TYR ASN LEU TYR ASP SER VAL ILE LYS ASN ILE GLN GLN PHE K1311 E1312 K1313 S1314 W1315 Q1316 D1317 V1318 S1319 K1320
D1321 D1322 L1323 A1324 K1325 M1326 E1327 E1328 D1329 ALA GLY LYS TYR GLY GLU GLN CYS SER ARG LEU PRO LYS ASP LEU LYS GLU TRP GLN ALA TYR ARG GLY LYS ASN LEU ASN LYS LEU TYR ASN LEU TYR ASP SER LEU ARG E1362 Q1363 L1364 P1365 L1366 I1367 I1368 S1369 L1370 K1371 S1374 I1375 M1376 P1377 R1378 H1379 K1382
I1383 K1384 E1385 I1386 T1387 N1388 T1389 K1390 Y1393 E1394 N1395 P1396 D1397 Q1398 F1399 Y1400 I1401 E1402 E1403 I1404 M1405 G1406 A1407 K1408 L1409 L1410 D1411 F1412 R1413 E1414 D1415 I1416 E1417 D1418 I1419 K1425 Q1426 L1427 L1433 Y1439 M1443 Q1444 F1445 Q1446 F1447 G1448 I1449 W1450 R1453 D1454 V1455 P1456 C1457
N1460 T1466 I1467 L1468 E1469 R1470 L1471 E1472 Q1475 L1476 Q1477 L1478 S1479 T1480 F1481 N1482 S1483 Q1484 R1485 H1486 V1487 T1488 K1491 A1492 L1497 F1501 V1504 N1505 D1506 W1518 L1521 E1522 P1523 T1526 G1527 G1528 A1531 R1532 A1538 K1539 Q1540 F1541 I1544 D1545 K1546 I1551 M1552
A1555 V1556 E1557 V1561 C1564 C1565 Q1566 N1567 D1568 M1569 D1572 L1581 E1582 D1583 C1584 Q1585 E1589 G1617 S1622 I1623 D1632 K1646 R1662 N1663 L1669 G1678 S1700 Q1704 K1734 V1735 R1741 A1749 M1750 K1753 R1754 N1755 E1756 I1757 K1758 E1759 H1760
M1761 N1762 I1763 L1764 S1765 L1769 E1770 D1771 L1772 R1778 C1800 K1801 D1802 V1803 N1804 D1805 F1806 E1807 W1808 D1819 I1820 I1827 T1828 A1841 Y1855 I1856 T1857 M1862 G1877 T1881 D1884 T1896 N1897 H1902 R1903 Q1916 S1917 G1918 D1924 E1925 I1929 D1930 L1931 E1932
V1933 L1934 S1935 I1944 I1964 E1965 V1970 S1971 Y1972 N1977 A1981 G1982 R1983 L1986 K1991 R1995 G1996 V1997 D2003 R2004 I2008 L2023 F2027 I2051 L2055 Q2064 E2065 I2066 L2074 D2115 V2116 I2120 I2124 N2132 S2164 T2175 K2176 L2177
G2178 S2179 P2180 H2181 I2185 I2203 D2206 G2210 V2211 T2214 E2242 N2243 L2244 V2247 L2248 D2249 E2273 A2317 K2322 L2323 G2324 N2325 I2326 L2327 R2328 K2329 F2336 I2337 Q2340 E2343 D2350 P2353 S2356 V2357 L2361 L2378 Q2381 G2397 I2398 Y2399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Q2595 K2603 Q2606 M2611 R2618 I2621 L2625 K2626 F2629 F2630 I2631 F2632 N2633 M2634 I2635 L2636 S2639 F2652 K2653 F2657 S2658 D2659 K2663 V2664 S2667 P2685 R2697 C2709 K2710 K2711 D2712 T2713 M2721 K2722 I2723 K2724 P2725 E2726 E2738 A2742 N2748
D2752 L2763 Q2768 I2769 E2770 K2776 Y2777 K2781 T2782 F2783 L2784 F2785 C2786 D2787 F2788 L2789 R2790 P2791 D2792 N2795 E2796 D2797 G2798 I2799 I2800 E2801 E2802 E2803 A2804 P2805 K2806 I2807 Y2808 E2809 A2810 I2811 D2812 S2813 L2824 R2831 K2836 V2840 D2843 D2844 A2845 L2846 K2847 L2850
R2851 I2852 S2853 R2857 L2864 G2872 K2873 Q2874 T2877 R2878 I2883 G2884 I2888 Q2889 Q2890 I2891 T2894 K2895 T2896 D2901 F2910 D2911 D2912 A2913 G2914 K2918 Q2919 L2923 M2924 T2925 E2928 V2929 K2930 K2931 E2932 E2933 F2934 L2935 E2936 Y2937 I2938 N2939 M2940 V2941 L2942 S2943 T2944 G2945
E2946 L2951 A2952 K2953 D2954 E2957 V2958 W2959 A2966 G2974 N2975 I2976 D2977 P2978 P2979 R2990 V2991 R2992 F3019 N3020 T3023 I3024 E3033 S3037 V3038 A3039 E3040 T3041 F3042 I3043 K3044 N3045 F3046 D3047 K3052 Q3057 M3069 I3073 C3074 F3092 Y3095 S3098 L3102
E3105 K3106 Y3107 D3108 Q3112 Q3113 S3116 F3117 L3121 I3124 Q3125 E3126 A3127 T3128 I3129 T3130 I3131 ASN GLN MET GLU ILE SER LEU LYS GLU GLU GLU ILE GLN LEU ASN GLU ALA THR GLU LYS THR ASN GLN LEU LEU ALA ASN LEU ASP LYS GLU SER LYS LYS ALA ASN GLN LYS
GLY GLU GLU VAL ALA ALA THR ASN LYS GLN CYS GLU ILE GLN ALA GLU GLN ILE SER LYS GLU GLU GLU ILE GLN LEU ASN GLU GLU GLN CYS GLU ILE GLN ALA GLU GLN ILE SER LYS GLU GLU GLU ARG GLU LEU GLU ALA ALA LEU PRO ALA LEU ARG ARG ALA GLN GLU ALA VAL ASP SER ILE GLU GLU SER LYS ASP ILE VAL GLU GLU LEU LYS ALA ASN LYS PRO
LEU ASP ILE ILE LYS TYR ILE MET ASP ALA VAL LEU VAL PHE PHE LYS ALA ARG LEU ILE PRO ILE GLN ILE GLU GLU ARG VAL PHE ASN LYS LYS GLU GLY LYS ALA VAL LEU PHE LEU LYS GLU SER TYR ASP GLU SER GLY ILE GLN THR LEU GLY ASP MET ASN PHE MET LYS LYS
LEU LYS GLU PHE GLU LYS ASP SER ILE ASN GLU GLU THR ILE GLU LEU LEU GLU PRO TYR LEU ASN GLN SER GLU ASP TRP PHE ASN ASP THR PHE ALA THR LYS ALA SER LYS ALA ALA ALA GLY ILE LEU LYS TRP ALA PHE ALA ILE TYR GLU TYR HIS GLN LYS SER LYS ILE VAL
LYS PRO LYS ARG ILE GLN VAL ALA ILE ALA GLU GLY ARG GLN ALA ILE ALA LEU LYS GLU LEU GLU LYS ALA ARG GLU ASP LEU ALA GLN ILE GLN ALA TYR ILE LYS ASN LEU LYS ASP VAL TYR THR LYS GLN MET GLU GLU LYS ASN GLU LEU GLU MET LYS ALA ALA LYS THR LYS
LYS LYS ILE ASN THR ALA ARG T3417 L3418 T3419 T3420 S3421 L3422 S3423 G3424 E3425 K3426 D3427 R3428 W3429 G3432 A3433 Q3434 D3438 Q3439 K3440 R3441 K3442 L3443 V3444 V3447 T3451 A3452 F3453 Y3456 Y3464 L3468 A3469 Q3470 Q3471 R3472 F3473 V3474 V3475 V3482 P3483 L3488 S3492 F3493 L3494
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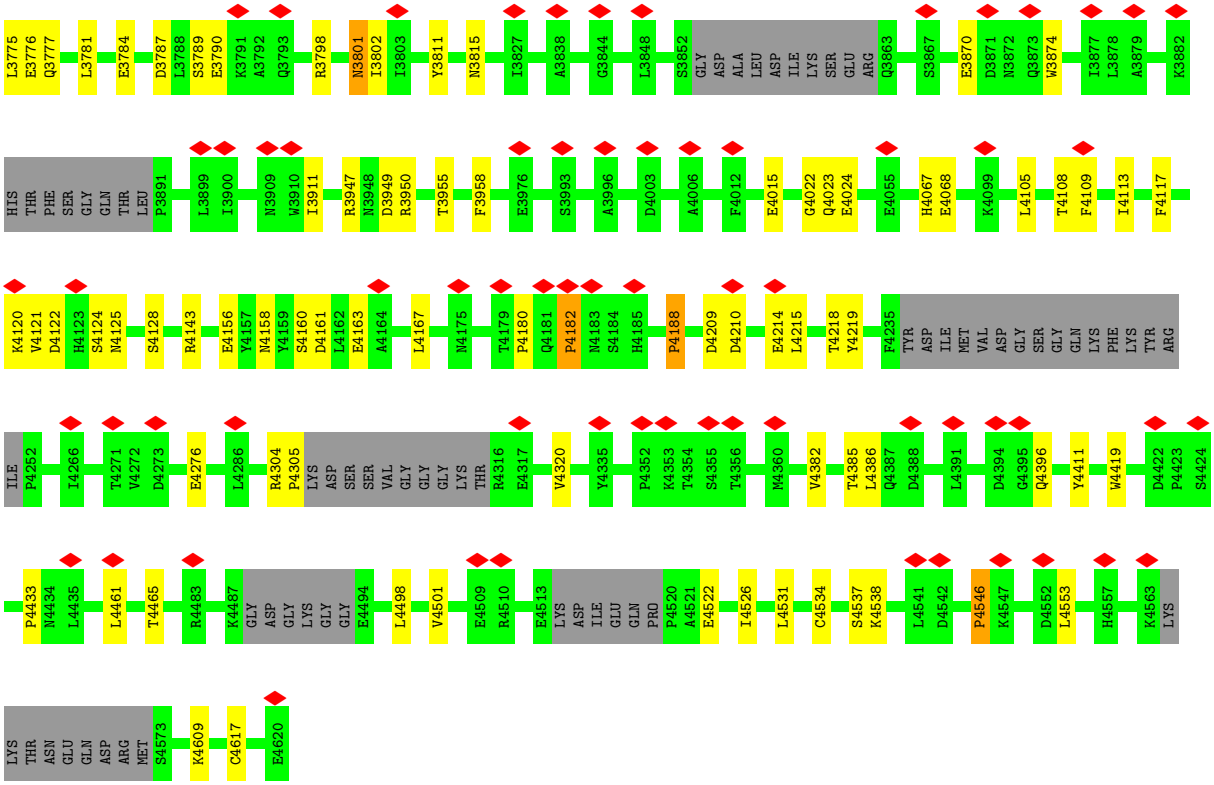
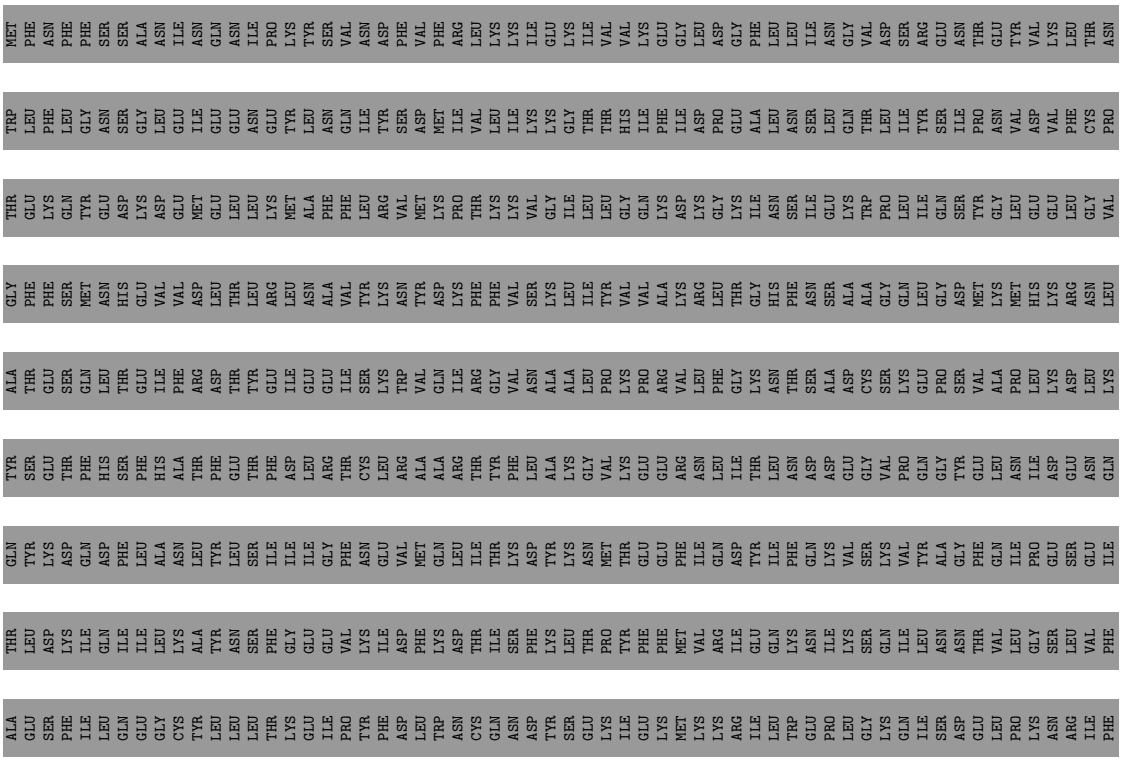
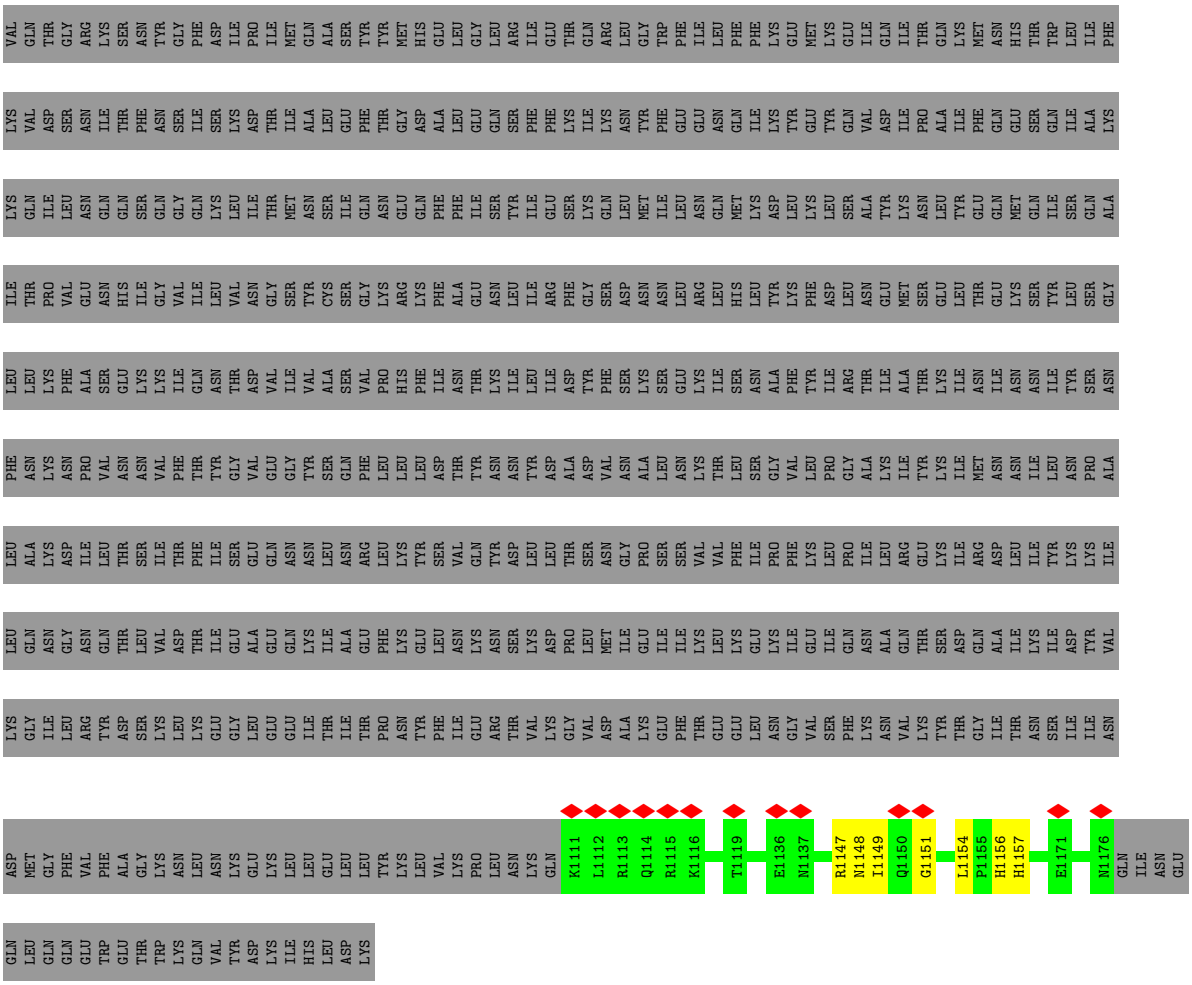
M3590 M3591 D3592 P3593 V3594 L3595 E3596 ARG GLN ILE ILE VAL LYS GLY LYS THR GLN PHE VAL ASN VAL ALA GLY THR GLU MET GLU L3617 E3620 L3623 F3624 M3625 T3626 C3627 R3628 P3636 E3637 L3638 S3639 A3640 K3641 I3645 D3646 T3650 L3654 L3658 L3659 S3664 K3665 E3666 Q3667 K3668
A3669 L3670 E3671 D3672 S3673 L3674 Q3683 N3684 Q3689 K3693 N3694 E3697 R3698 L3699 I3700 N3701 S3702 Q3703 G3704 N3705 L3706 L3707 D3708 D3709 T3710 E3711 L3712 M3713 D3714 V3715 T3719 K3720 T3721 Q3722 V3726 A3727 A3728 K3729 L3730 N3741 R3744 E3745 Q3746 Y3747 R3748 L3766 M3770 Y3771 N3772



• Molecule 2: Shulin

Chain Y: 5% 94%

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R1113
Q1114
R1115
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E1136
N1137
R1147
N1148
I1149
Q1150
G1151
L1154
P1155
H1156
H1157
E1171
N1176

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49397	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	499.5, 499.5, 499.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.37	1/22277 (0.0%)	0.65	18/30197 (0.1%)
2	Y	0.37	0/477	0.60	0/648
All	All	0.37	1/22754 (0.0%)	0.65	18/30845 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2857	ARG	CB-CG	-5.58	1.37	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2857	ARG	NE-CZ-NH2	-25.58	107.51	120.30
1	C	2857	ARG	NH1-CZ-NH2	8.53	128.78	119.40
1	C	3069	MET	CB-CG-SD	-7.32	90.44	112.40
1	C	3069	MET	CG-SD-CE	-6.80	89.32	100.20
1	C	4182	PRO	N-CA-CB	6.65	111.28	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	21875	0	20694	197	0
2	Y	466	0	390	5	0
3	C	81	0	36	0	0
4	C	31	0	12	0	0
All	All	22453	0	21132	202	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 5.

The worst 5 of 202 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:C:2499:LYS:NZ	1:C:2611:MET:O	2.11	0.83
1:C:1314:SER:O	1:C:1318:VAL:N	2.14	0.79
1:C:4125:ASN:O	1:C:4128:SER:OG	2.00	0.77
1:C:2776:LYS:O	1:C:2781:LYS:NZ	2.18	0.76
1:C:3636:PRO:O	1:C:3639:SER:OG	2.03	0.74

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	C	2877/4620 (62%)	2606 (91%)	265 (9%)	6 (0%)	47 81
2	Y	64/1200 (5%)	55 (86%)	9 (14%)	0	100 100
All	All	2941/5820 (50%)	2661 (90%)	274 (9%)	6 (0%)	50 81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2978	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2979	PRO
1	C	4182	PRO
1	C	4188	PRO
1	C	4546	PRO

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	C	2182/4196 (52%)	2179 (100%)	3 (0%)	93 97
2	Y	33/1102 (3%)	33 (100%)	0	100 100
All	All	2215/5298 (42%)	2212 (100%)	3 (0%)	93 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2329	LYS
1	C	2748	ASN
1	C	3801	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	ADP	C	4703	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	4 (13%)
4	ATP	C	4702	-	26,33,33	0.87	1 (3%)	31,52,52	1.68	5 (16%)
3	ADP	C	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	3 (10%)
3	ADP	C	4704	-	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	4703	-	-	4/12/32/32	0/3/3/3
4	ATP	C	4702	-	-	4/18/38/38	0/3/3/3
3	ADP	C	4701	-	-	1/12/32/32	0/3/3/3
3	ADP	C	4704	-	-	3/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4704	ADP	C5-C4	2.25	1.46	1.40
3	C	4701	ADP	C5-C4	2.18	1.46	1.40
3	C	4703	ADP	C5-C4	2.13	1.46	1.40
4	C	4702	ATP	C5-C4	2.03	1.46	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	4702	ATP	PA-O3A-PB	-5.12	115.25	132.83
3	C	4701	ADP	PA-O3A-PB	-4.56	117.17	132.83
3	C	4704	ADP	PA-O3A-PB	-4.21	118.36	132.83
4	C	4702	ATP	PB-O3B-PG	-4.13	118.64	132.83
3	C	4703	ADP	PA-O3A-PB	-4.13	118.66	132.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

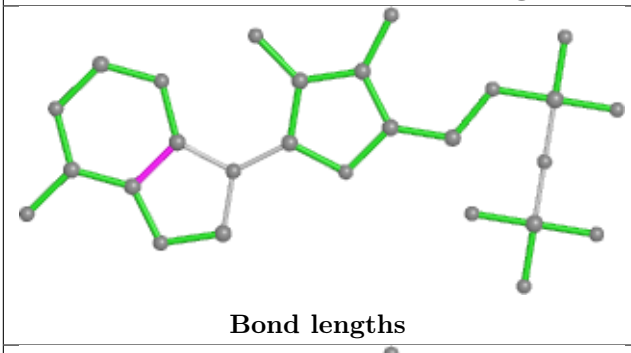
Mol	Chain	Res	Type	Atoms
3	C	4703	ADP	C5'-O5'-PA-O1A
3	C	4703	ADP	C5'-O5'-PA-O2A
3	C	4704	ADP	C5'-O5'-PA-O2A
4	C	4702	ATP	C5'-O5'-PA-O1A
4	C	4702	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

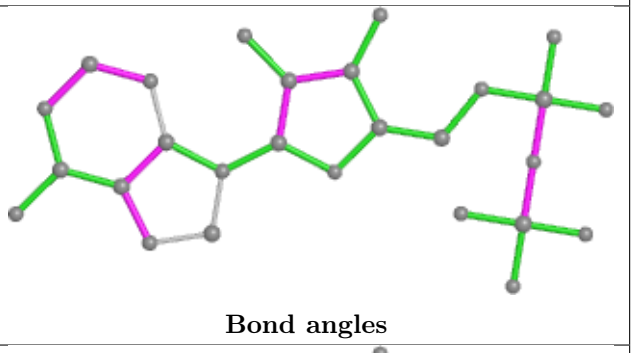
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

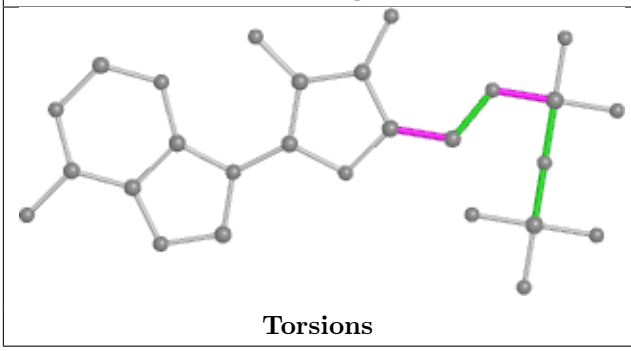
Ligand ADP C 4703



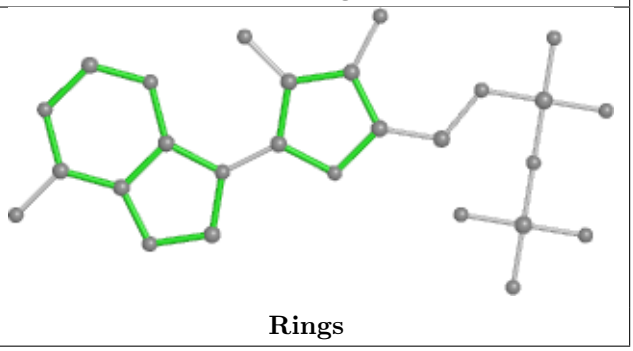
Bond lengths



Bond angles

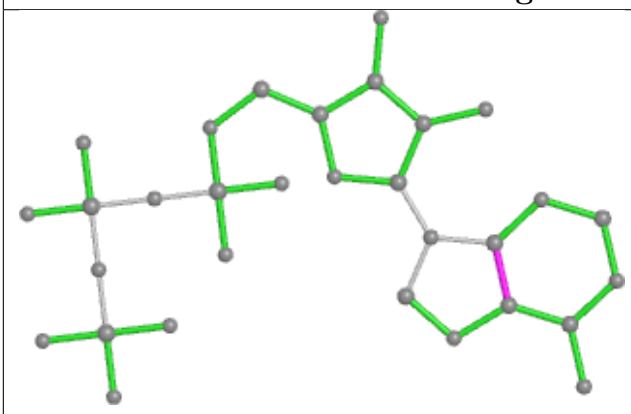


Torsions

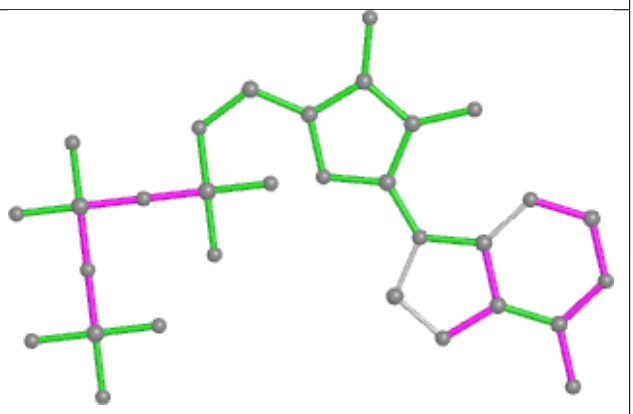


Rings

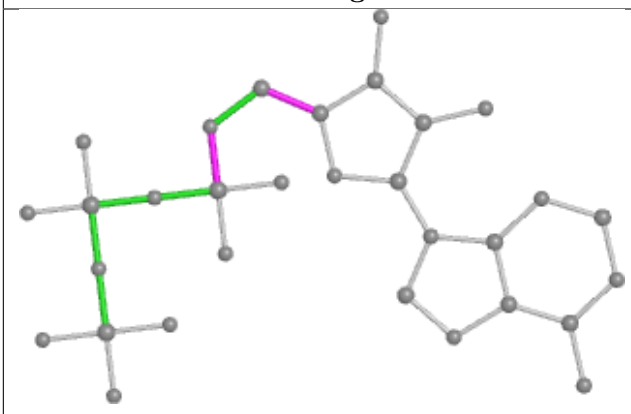
Ligand ATP C 4702



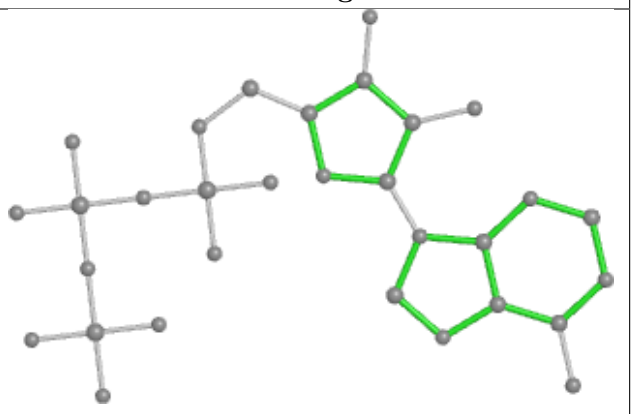
Bond lengths



Bond angles

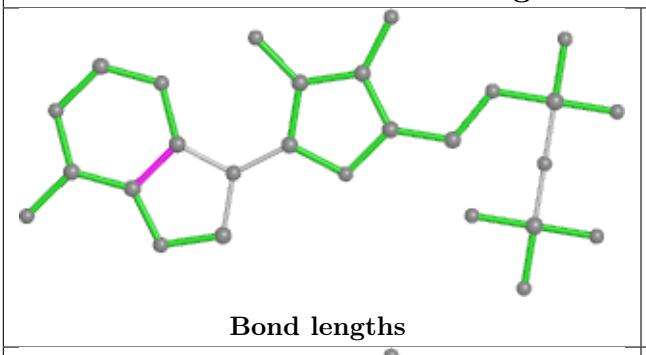


Torsions

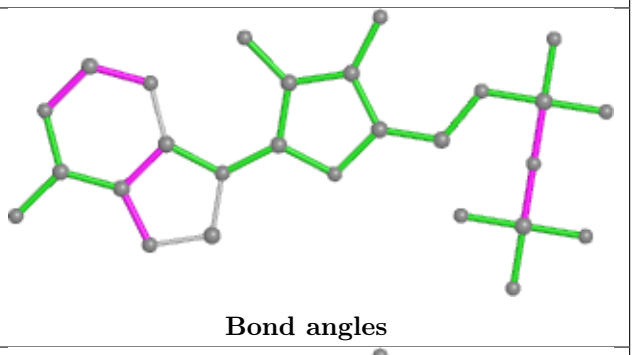


Rings

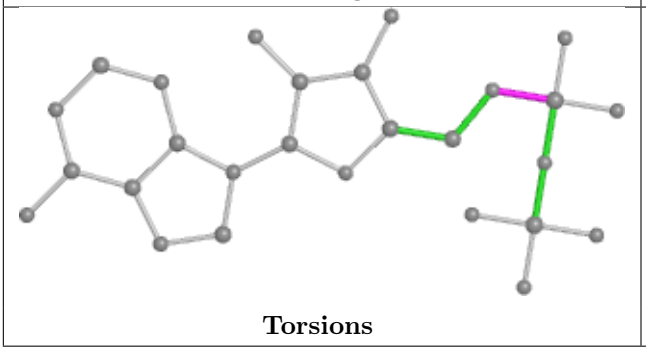
Ligand ADP C 4701



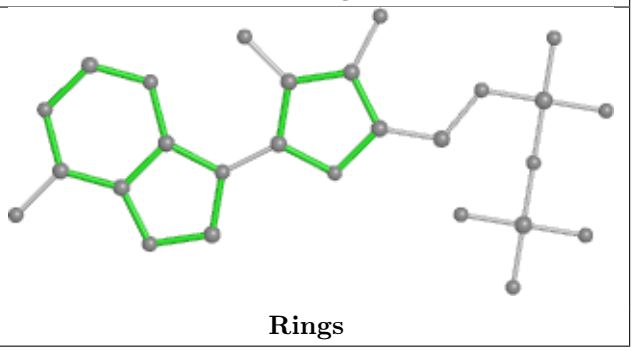
Bond lengths



Bond angles

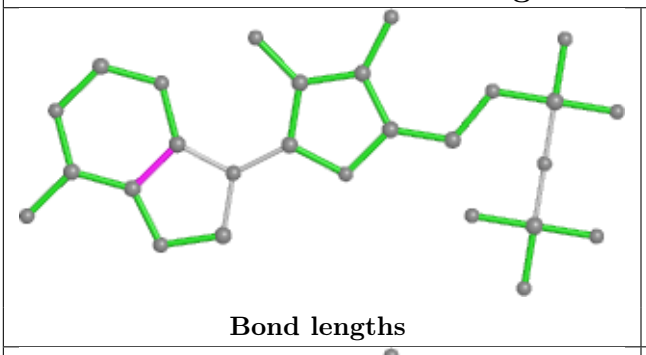


Torsions

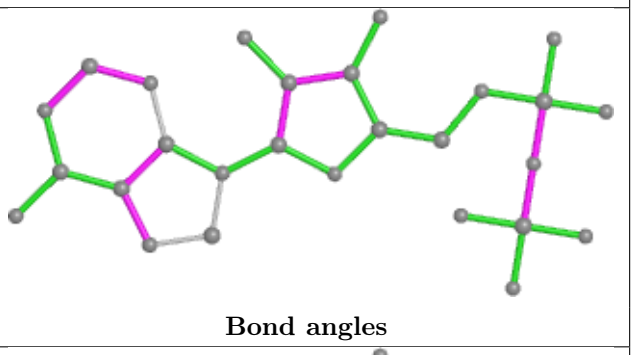


Rings

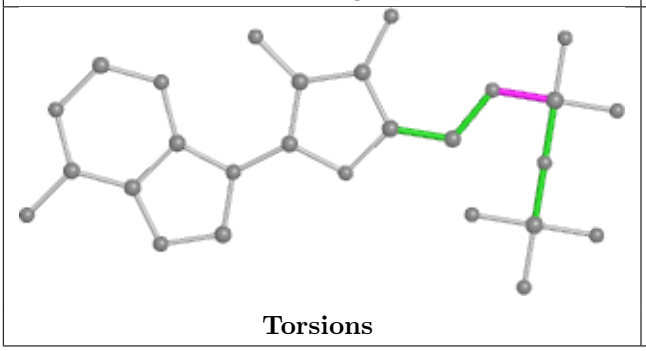
Ligand ADP C 4704



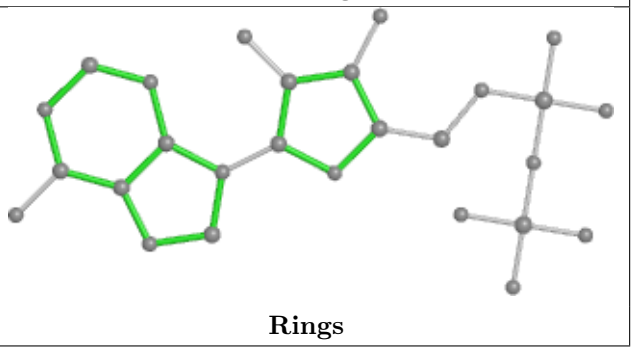
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

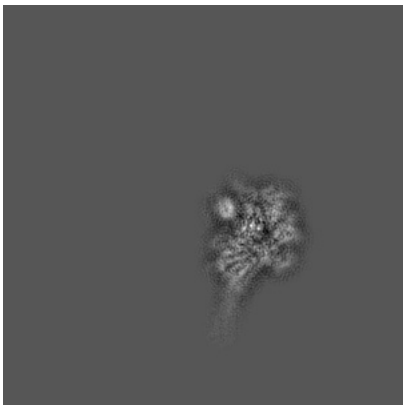
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11581. These allow visual inspection of the internal detail of the map and identification of artifacts.

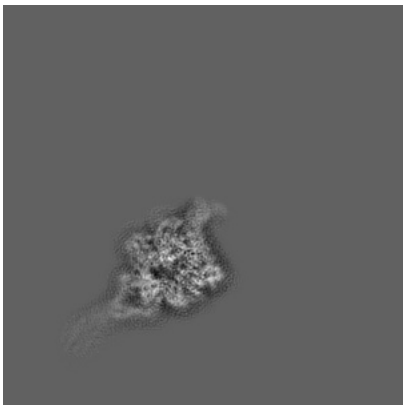
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

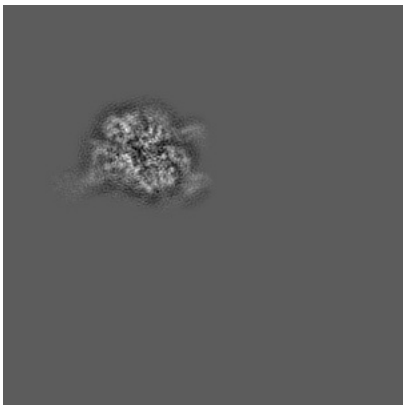
6.1.1 Primary map



X

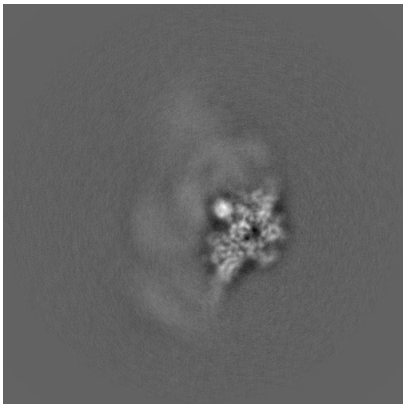


Y

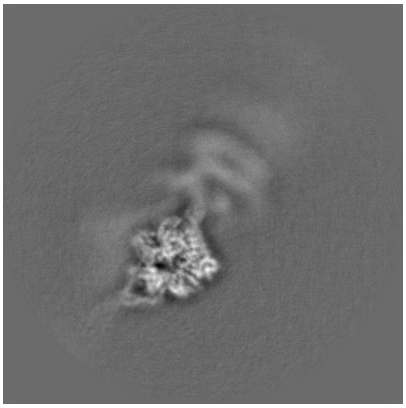


Z

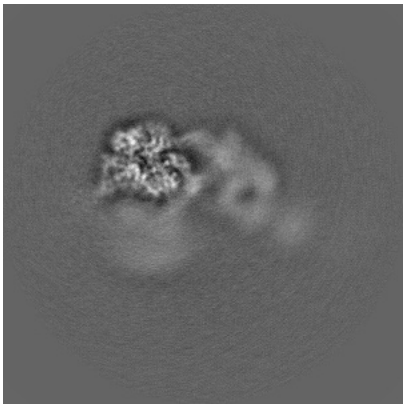
6.1.2 Raw map



X



Y

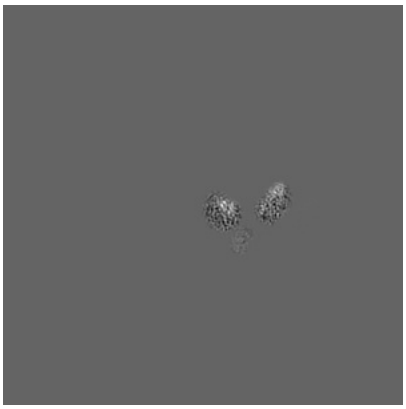


Z

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

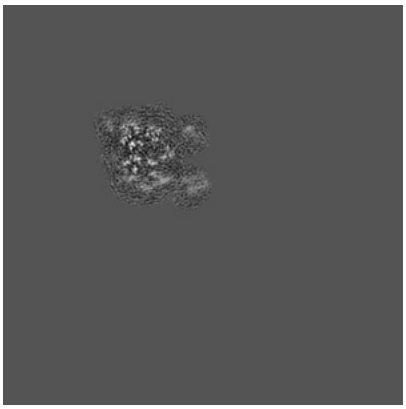
6.2 Central slices (i)

6.2.1 Primary map



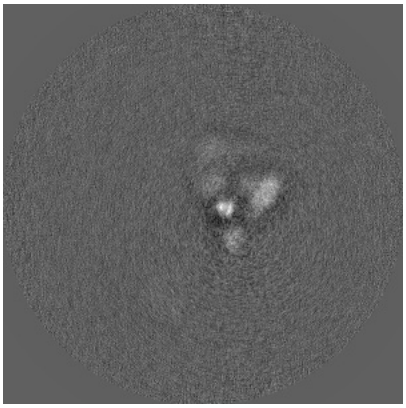
X Index: 225

Y Index: 225

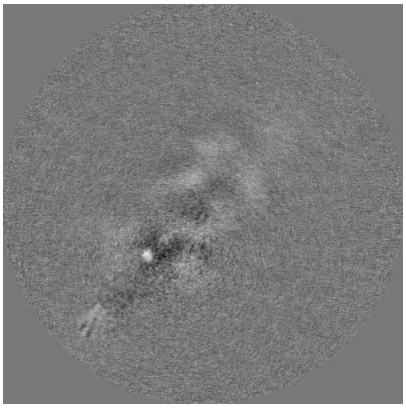


Z Index: 225

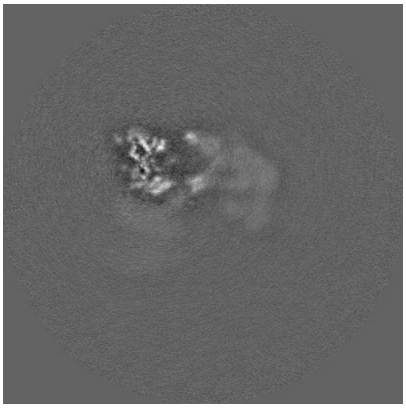
6.2.2 Raw map



X Index: 256



Y Index: 256

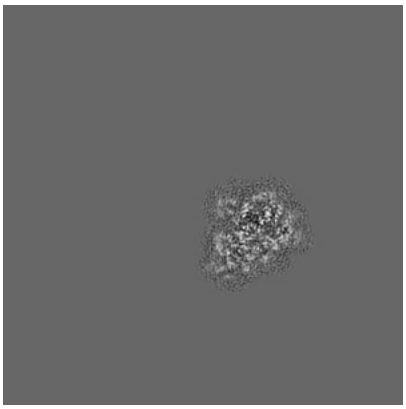


Z Index: 256

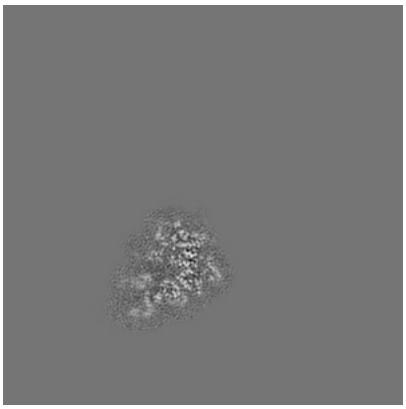
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

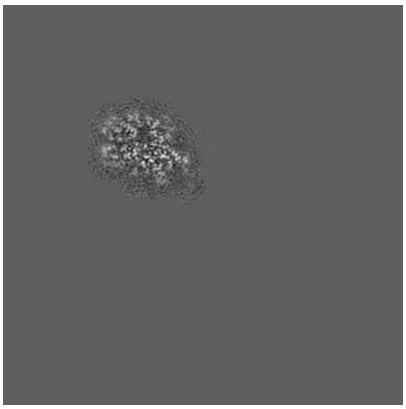
6.3.1 Primary map



X Index: 164

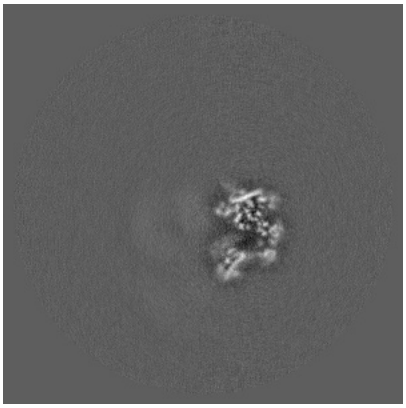


Y Index: 281

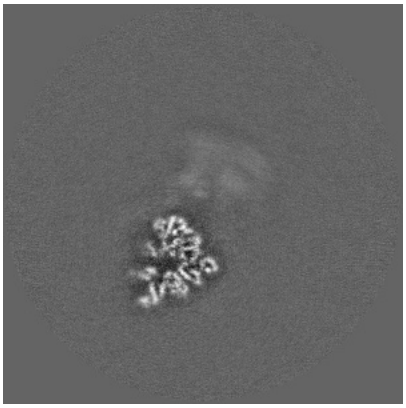


Z Index: 201

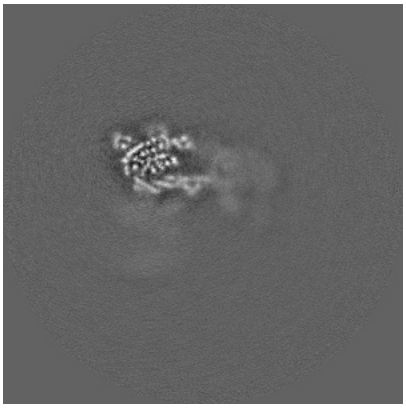
6.3.2 Raw map



X Index: 171



Y Index: 305



Z Index: 243

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

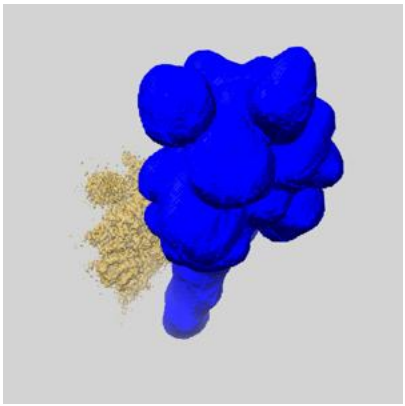
6.5 Mask visualisation (i)

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

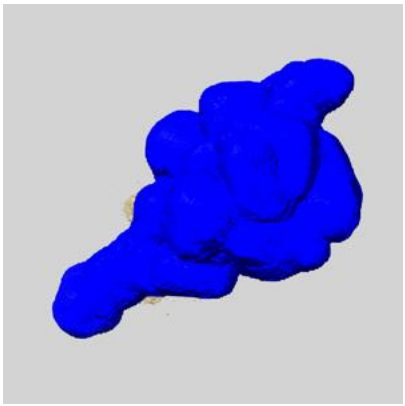
A mask typically either:

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

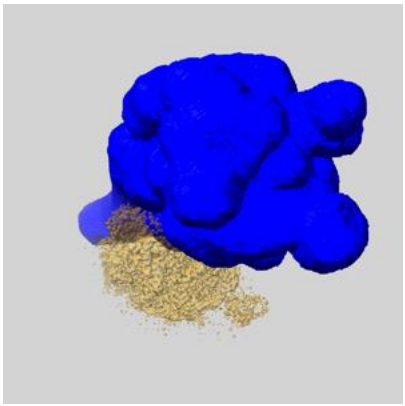
6.5.1 emd_11581_msk_2.map (i)



X

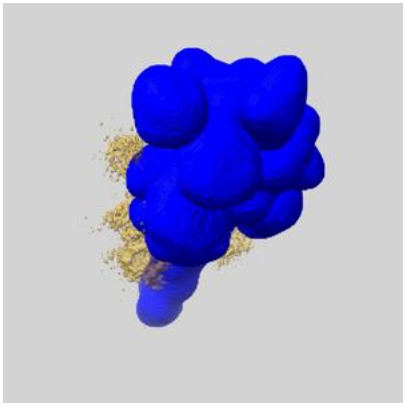


Y

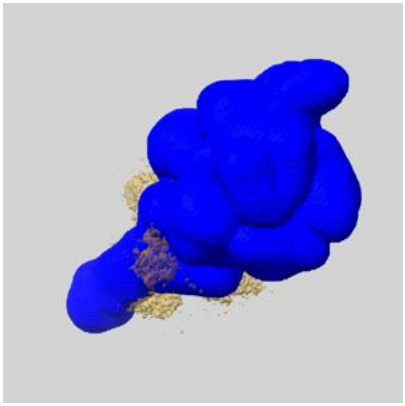


Z

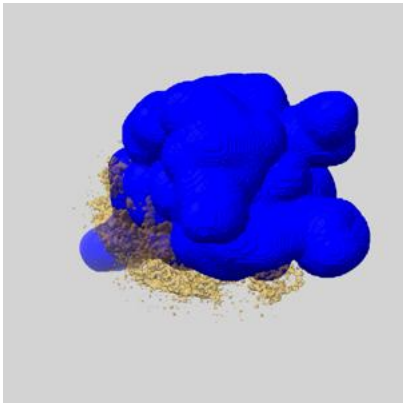
6.5.2 emd_11581_msk_1.map (i)



X



Y

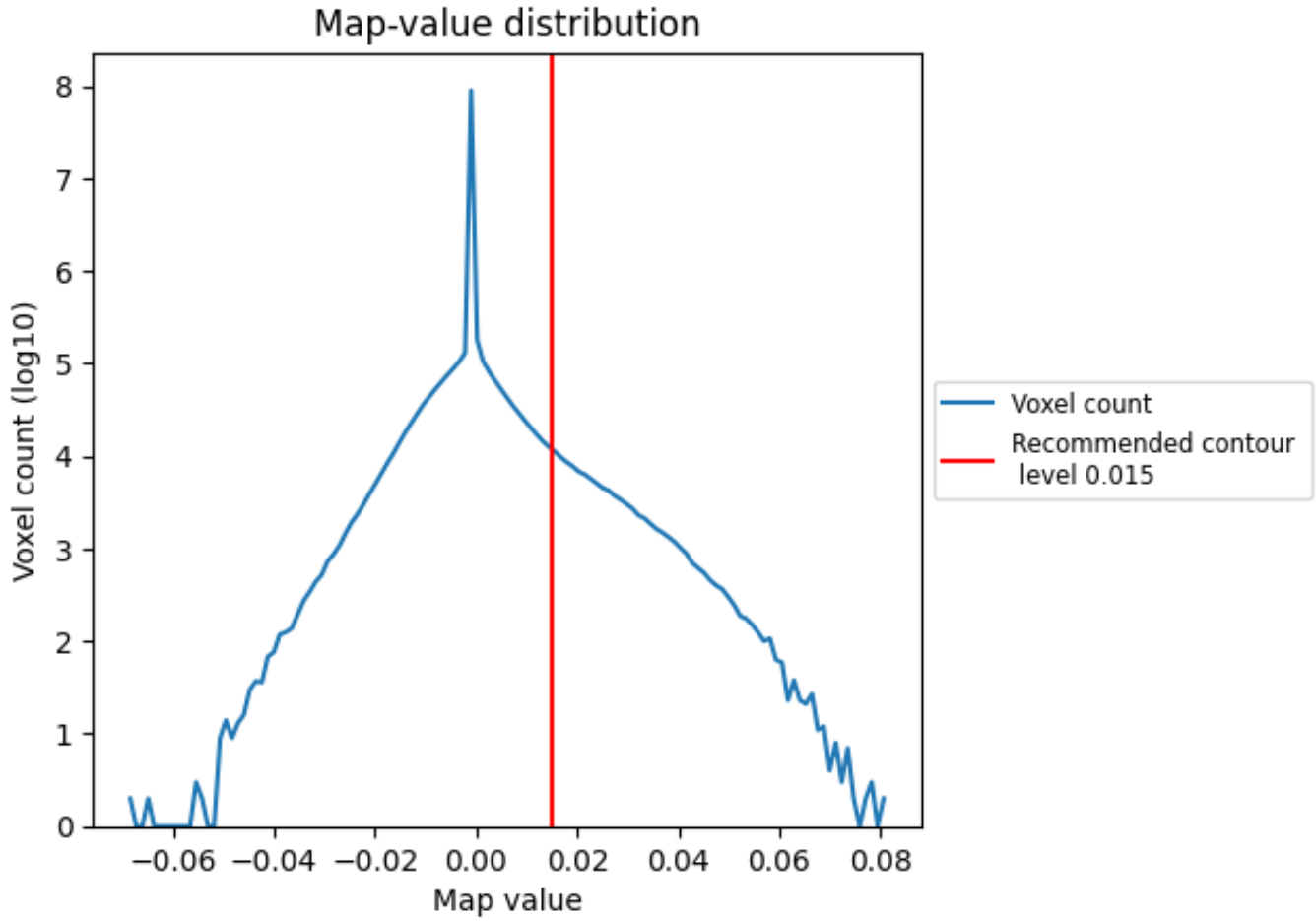


Z

7 Map analysis

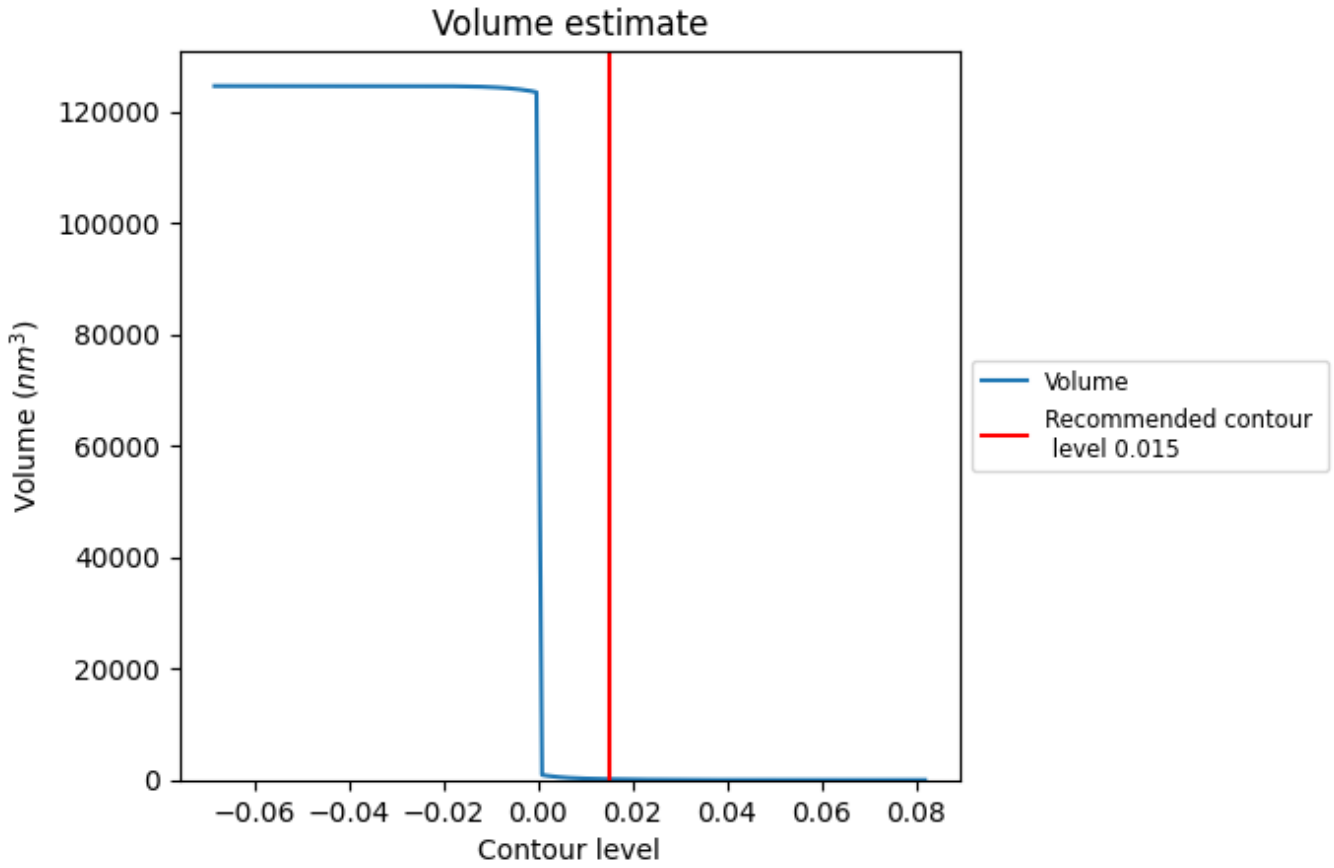
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

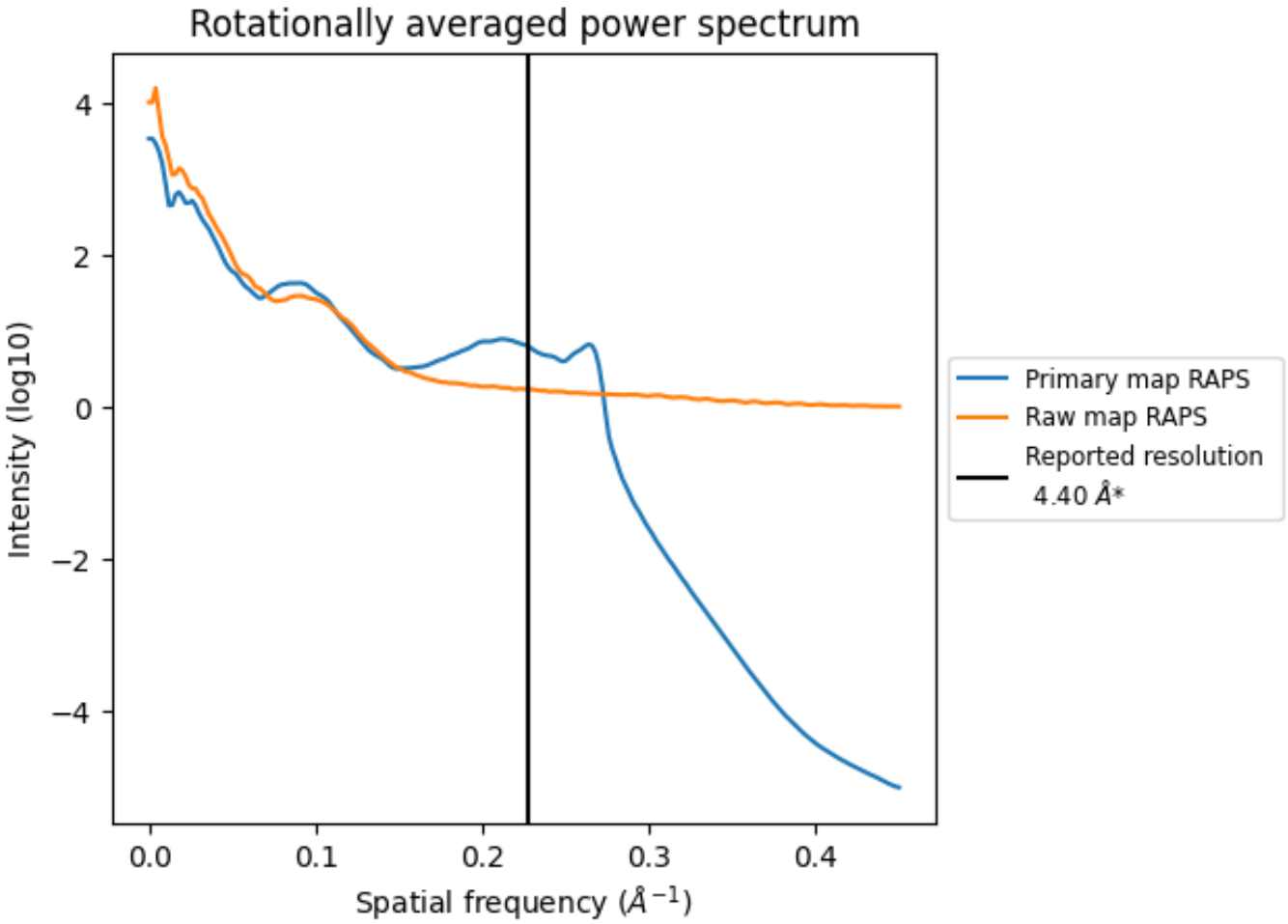
7.2 Volume estimate (i)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

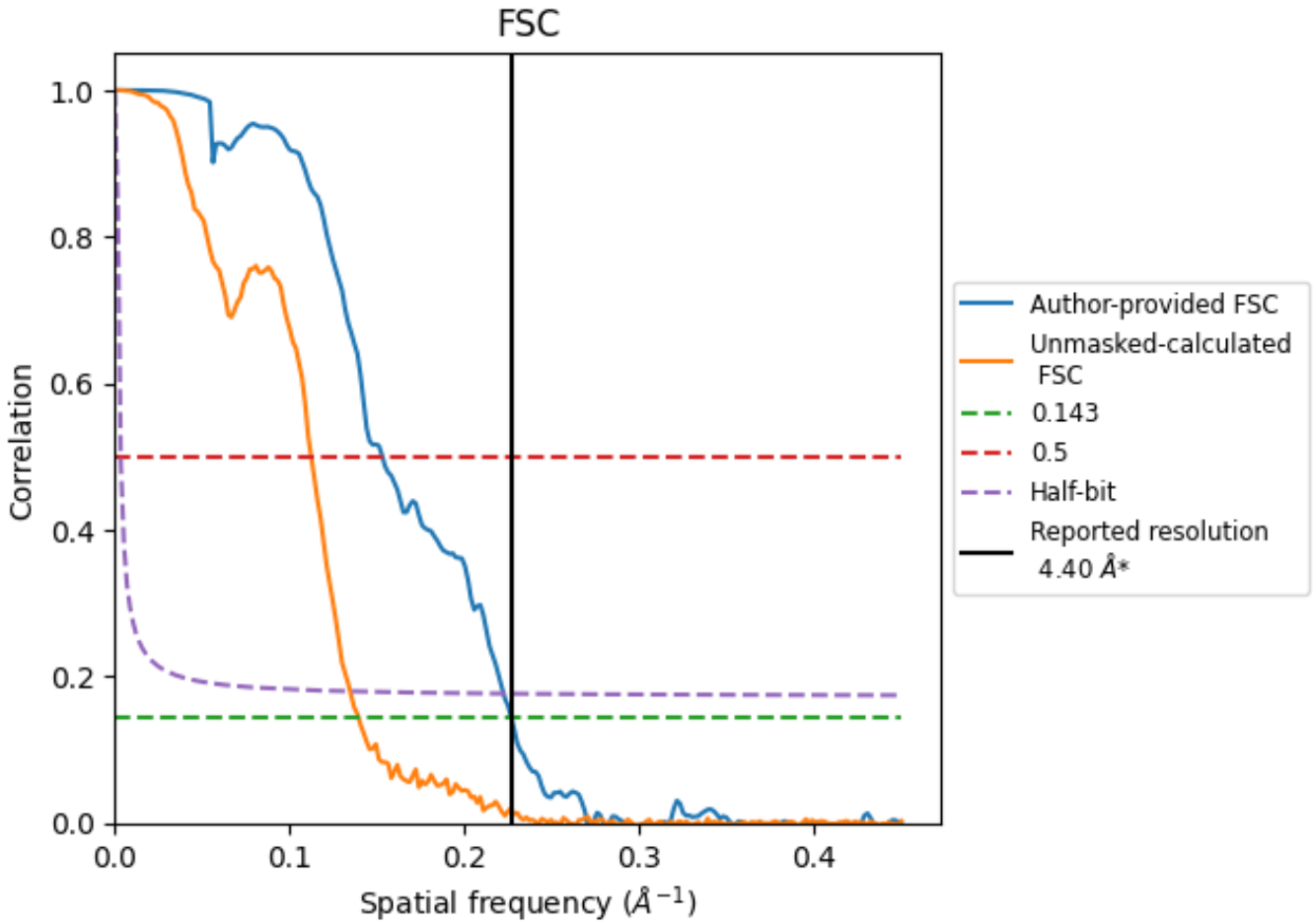


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

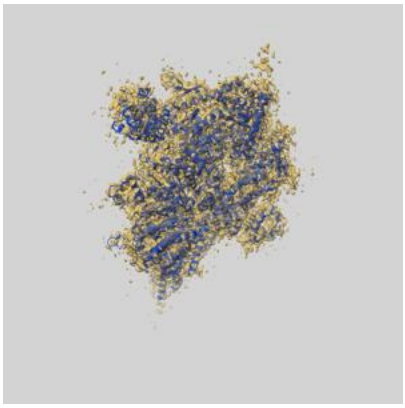
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	6.53	4.49
Unmasked-calculated*	7.16	8.88	7.42

*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 7.16 differs from the reported value 4.4 by more than 10 %

9 Map-model fit

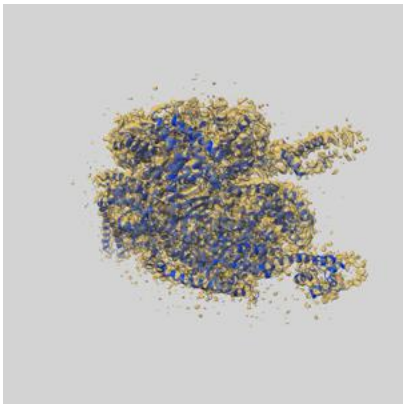
This section contains information regarding the fit between EMDB map EMD-11581 and PDB model 6ZYY. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay



X

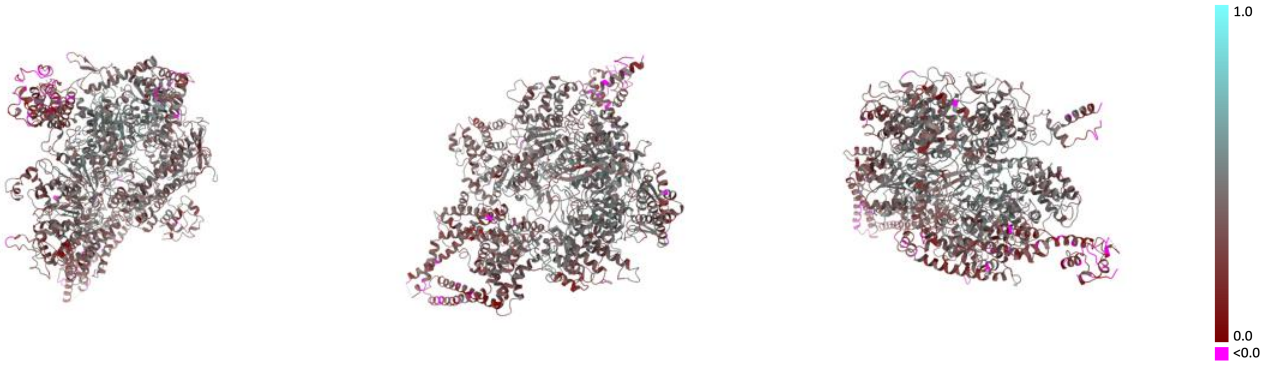
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

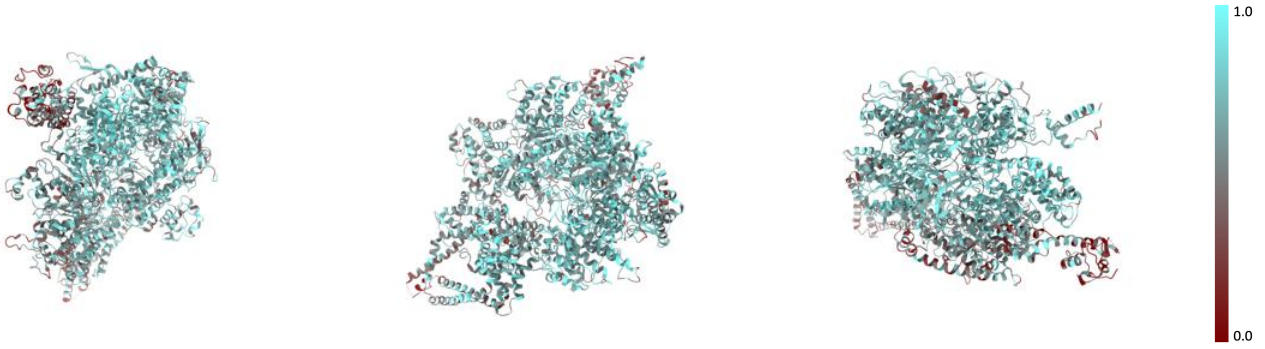
9.2 Q-score mapped to coordinate model



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.

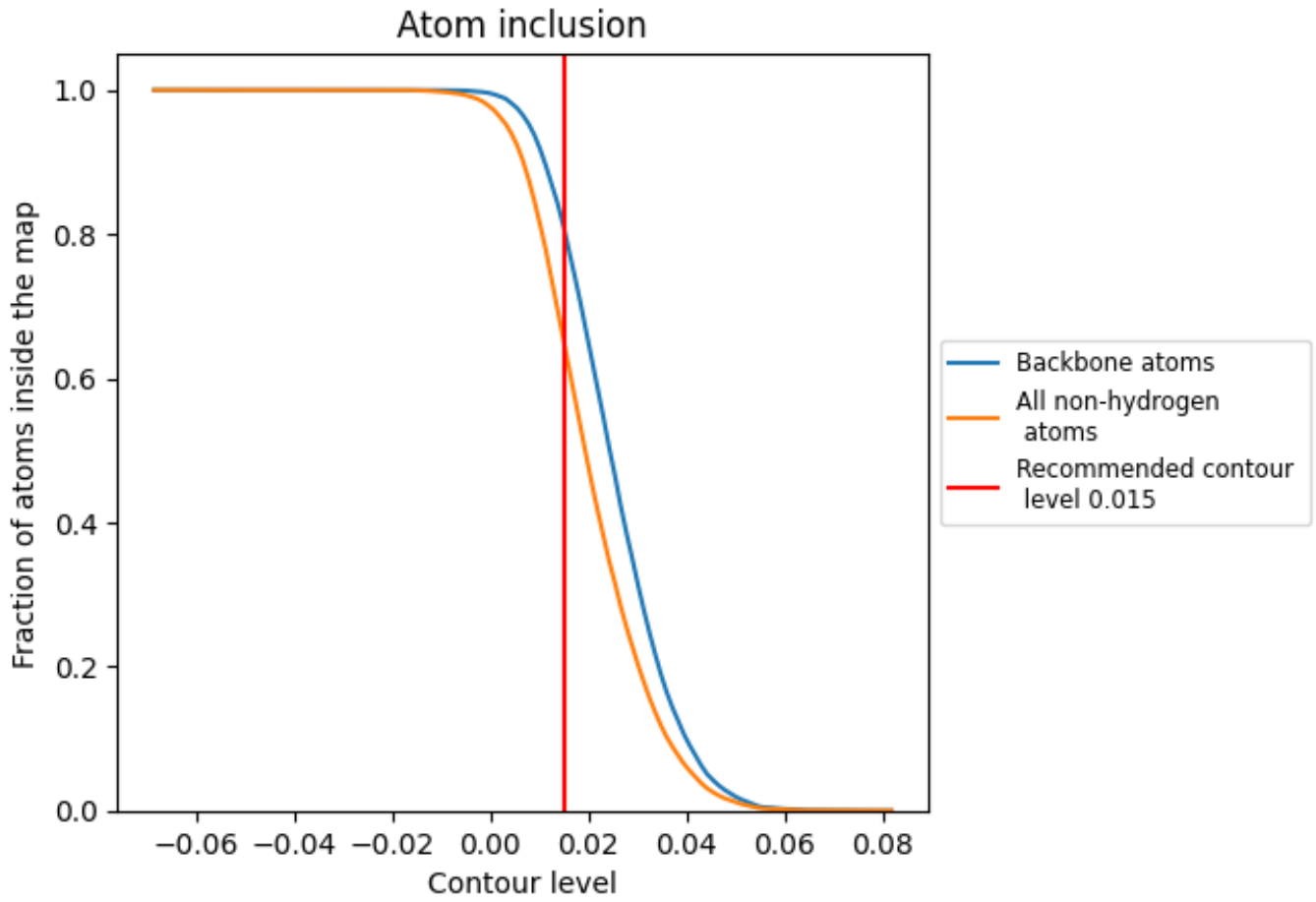
9.3 Atom inclusion mapped to coordinate model



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 65% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6542	0.3880
C	0.6546	0.3890
Y	0.6368	0.3590