wwPDB EM Validation Summary Report ⓘ

Apr 2, 2024 – 11:18 pm BST

PDB ID	:	8PQY
EMDB ID	:	EMD-17828
Title	:	Cytoplasmic dynein-1 motor domain bound to LIS1
Authors	:	Singh, K.; Lau, C.K.; Manigrasso, G.; Gassmann, R.; Carter, A.P.
Deposited on	:	2023-07-12
Resolution	:	3.80 Å(reported)
Based on initial model	:	7Z8G

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 ⓘ 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:

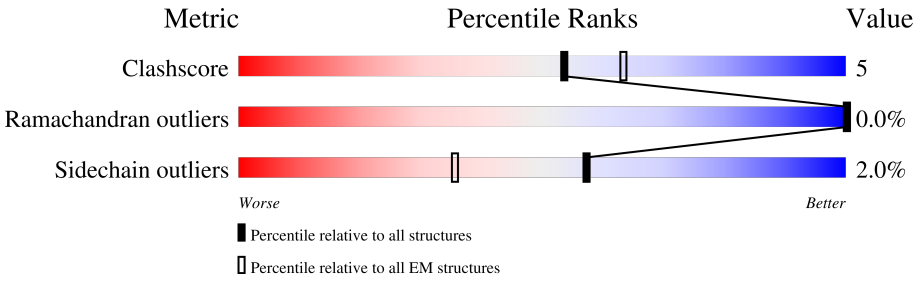
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	A	4646	5% 53% 9% 38%
2	B	410	8% 61% 14% · 24%
2	C	410	9% 57% 19% 24%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27916 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
1	A	2892	Total	C	N	O	S	0	0
			22814	14566	3940	4197	111		

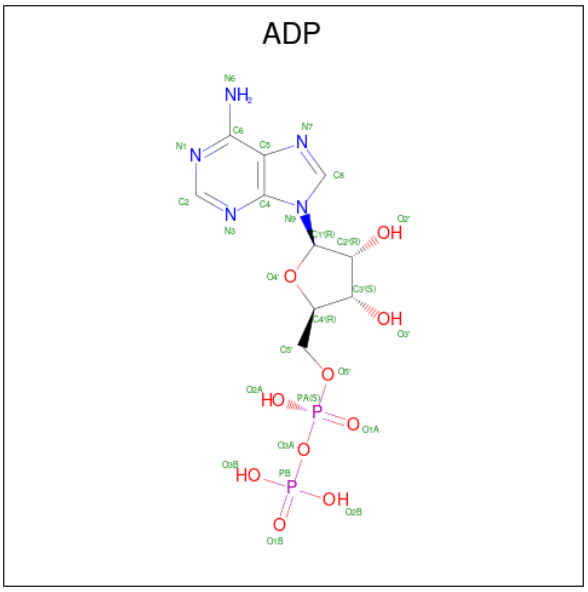
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1567	GLU	ARG	engineered mutation	UNP Q14204
A	1610	GLU	LYS	engineered mutation	UNP Q14204

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	313	Total	C	N	O	S	0	0
			2494	1571	440	463	20		
2	C	313	Total	C	N	O	S	0	0
			2494	1571	440	463	20		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

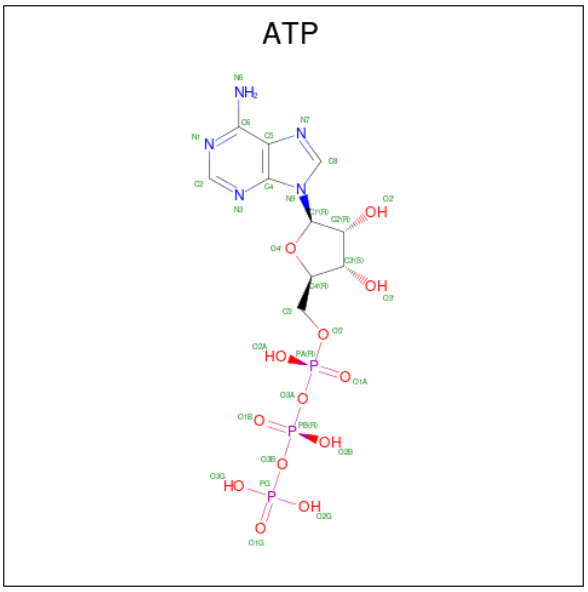


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



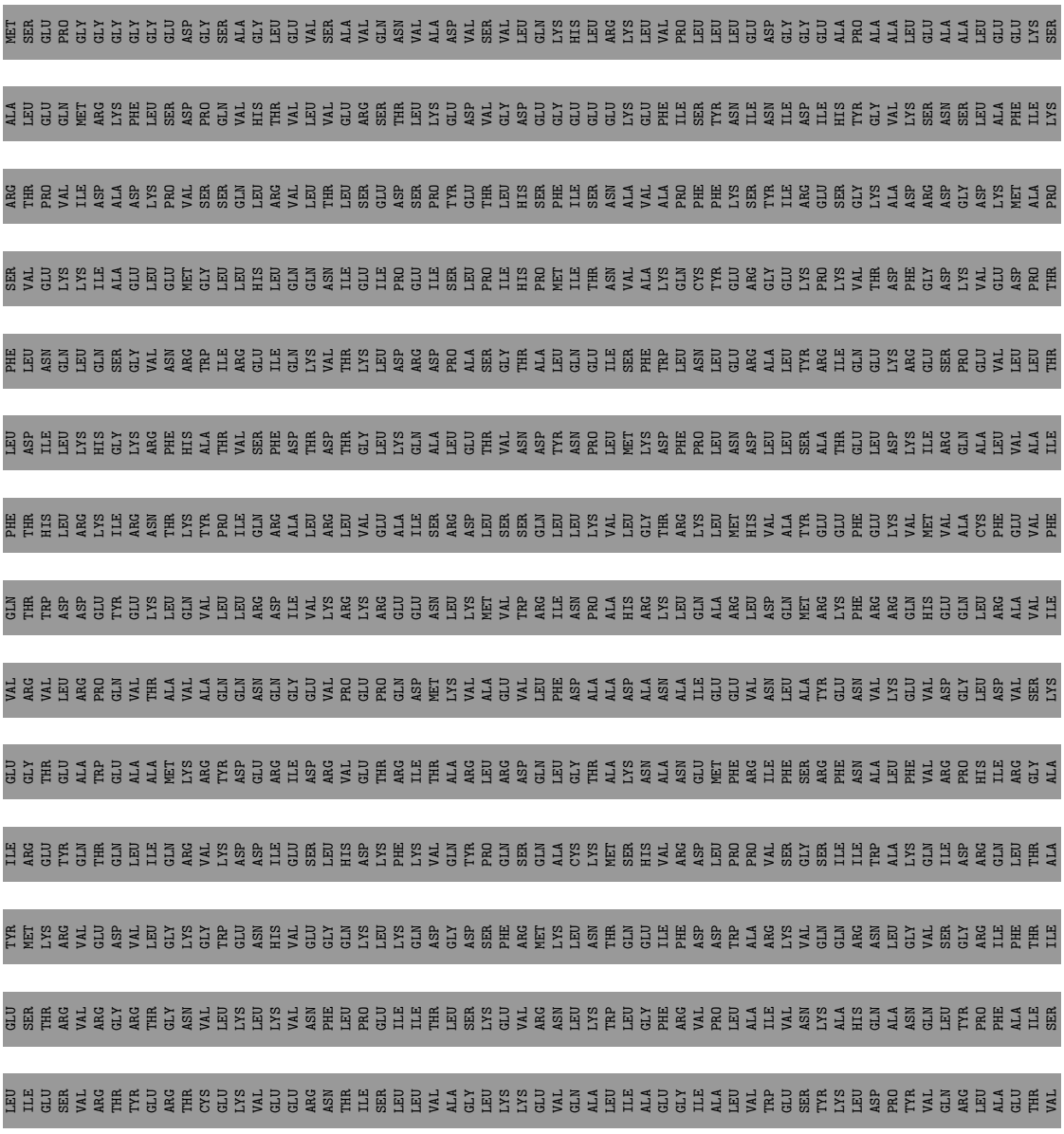
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

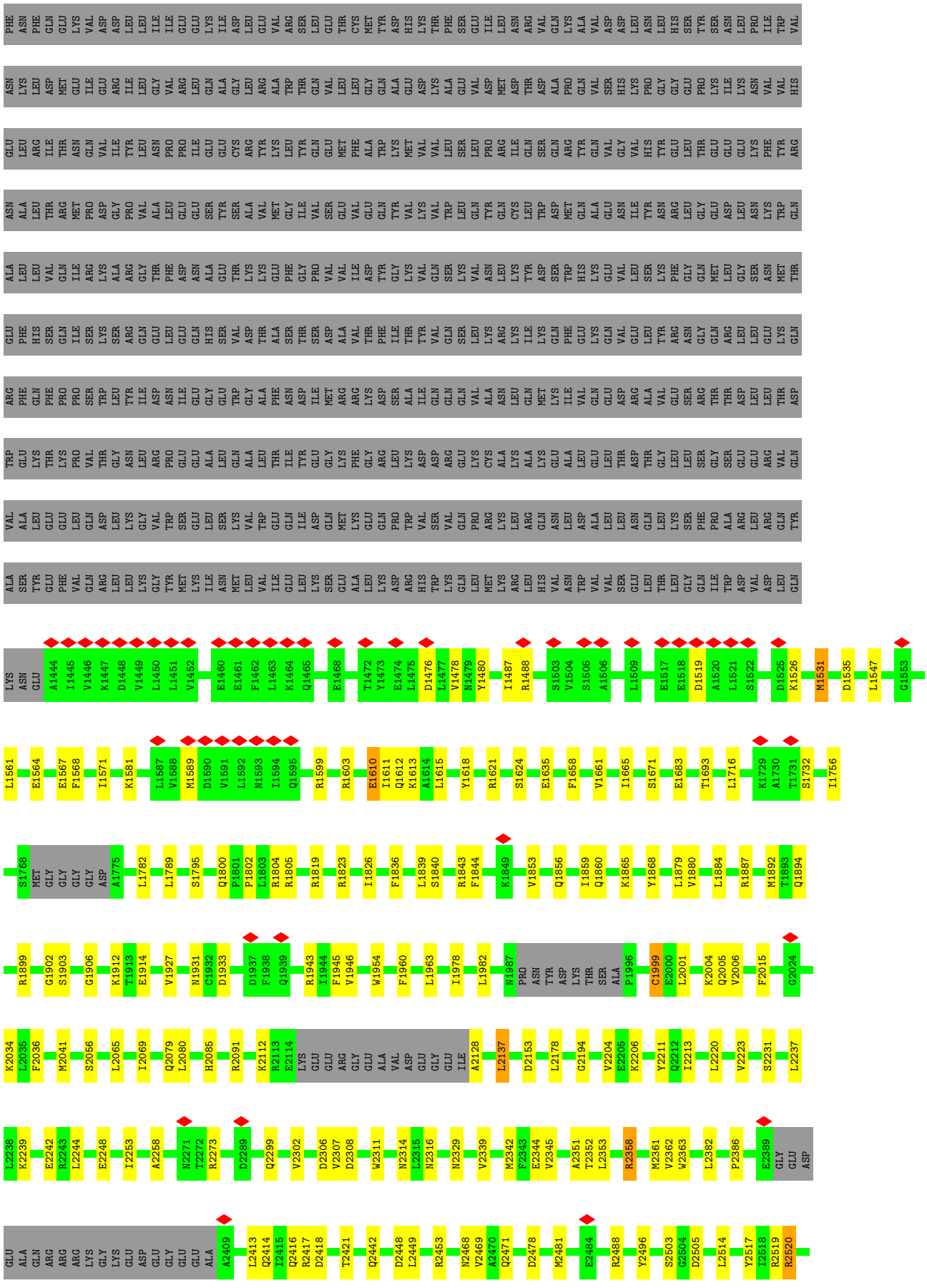
3 Residue-property plots (i)

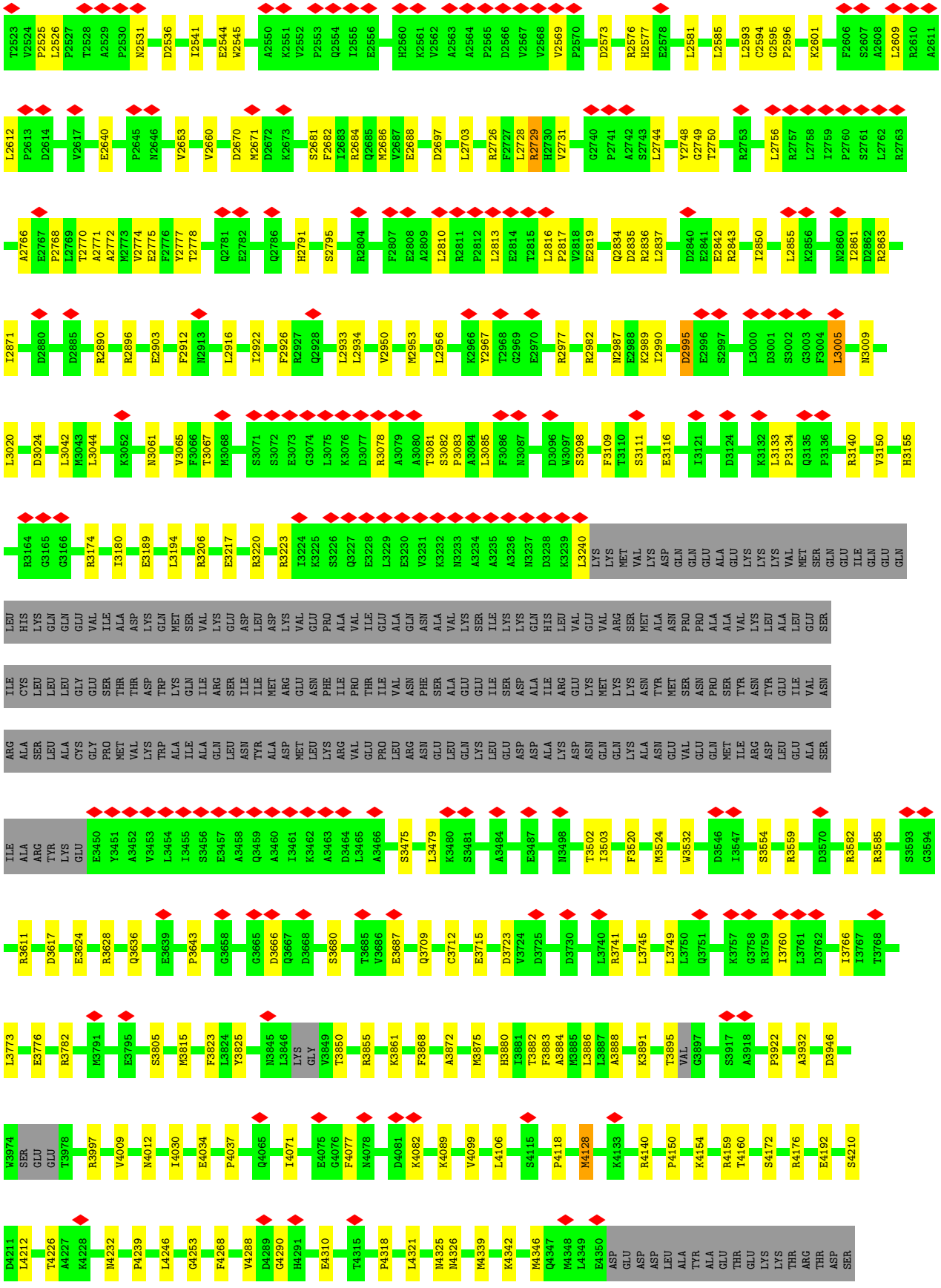
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

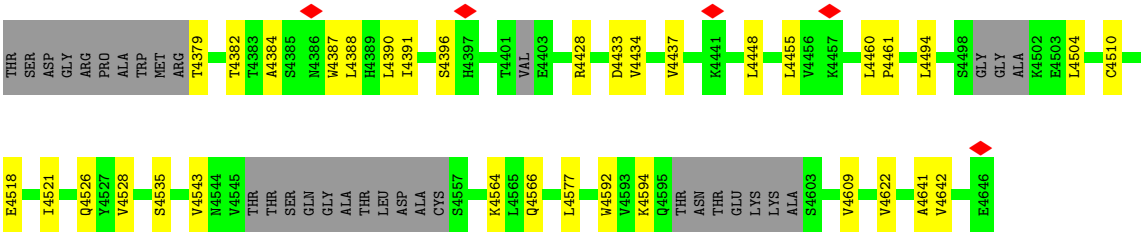
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain A:



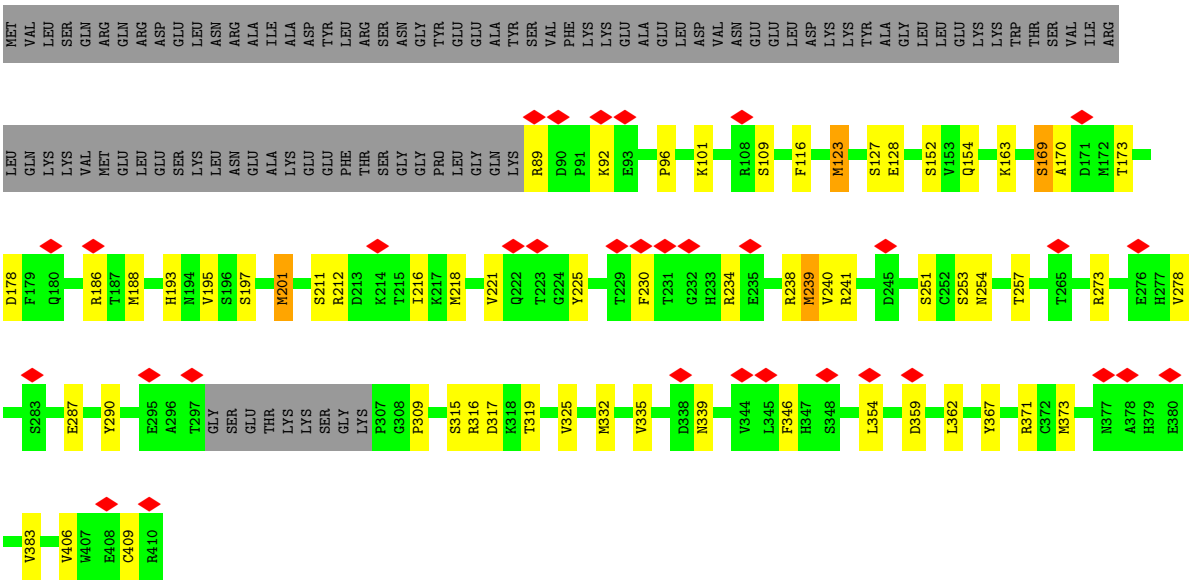

PHE ASN PHE GLN GLU LYS VAL ASP ASP LEU LEU ILE ILE GLU GLU LYS ILE ASP LEU GLU VAL ARG SER LEU GLU THR CYS MET TYR ASP HIS LYS THR PHE SER GLU ILE LEU ASN ARG VAL GLN LYS ALA VAL ASP ASP LEU ASN LEU LEU HIS SER TYR SER ASN LEU PRO ILE VAL VAL HIS
ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ARG LEU GLN ALA GLY LEU ARG ALA TRP THR GLN VAL LEU LEU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP MET ASP THR ASP ALA PRO GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS
GLU LEU ARG ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU GLU SER LEU PRO ARG ILE GLN SER GLN ASP MET GLN ARG TYR GLN VAL GLY VAL HIS TYR ASN ARG LEU GLY GLU GLU LYS PHE TYR ARG
ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER TYR SER ALA VAL MET GLY ILE VAL SER GLU VAL GLN LEU TRP SER LEU GLN TYR GLN CYS LEU TRP ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS TRP GLN
ALA LEU LEU VAL GLN ILE ARG LYS ALA ARG GLY THR PHE ASP ASN ALA GLU THR LYS LYS GLU PHE GLY PRO VAL VAL ILE ASP TYR GLY LYS VAL GLN SER LYS VAL LEU ASN LEU LYS TYR ASP SER TRP HIS LYS GLU VAL LEU SER LYS PHE GLY GLN MET LEU GLY SER ASN MET THR
GLU PHE HIS SER GLN ILE SER LYS SER ASP ALA VAL THR PHE ILE THR TYR VAL GLN LEU GLU LEU TYR ARG GLN GLU LYS GLN VAL GLY GLN VAL GLU LEU TYR ARG ASN GLY GLN LEU ARG LEU GLU LYS ARG ILE LYS GLN PHE GLU LYS GLN VAL GLU VAL ASP LEU LEU GLU LYS
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ASP ILE MET ARG ARG LYS ASP SER ALA ILE ASP ASN LEU GLN MET LYS ILE VAL GLU ALA ASP ASP ALA VAL GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP LEU LEU THR ASP
TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU LEU ARG PRO GLU GLU ALA LEU LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LEU LEU GLU THR ASP THR GLY LEU GLY GLY SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU LEU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU GLN ILE ASP GLN MET LYS GLU GLN PRO TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN ASN LEU ASP ALA LEU LEU ASN GLN LEU LYS GLU ASN LEU ASP ARG GLN ALA VAL GLU SER PHE PRO ALA ARG LEU GLN ARG GLN TYR
ALA SER TYR GLU PHE VAL GLN ARG LEU LEU LYS LYS GLY TYR MET LYS ILE ASN MET LEU VAL ILE GLU LEU LYS SER GLU ALA LEU LYS ASP ARG HIS TRP LYS GLN LEU MET LYS ARG LEU HIS VAL ASN TRP VAL VAL SER GLU LEU THR LEU GLY GLN ILE TRP ASP VAL ASP LEU GLN
LYS ASN GLU A1444 I1445 V1446 K1447 D1448 V1449 L1450 L1451 V1452 E1460 E1461 F1462 L1463 K1464 Q1465 E1468 T1472 Y1473 E1474 L1475 D1476 L1477 V1478 N1479 Y1480 I1487 R1488 S1503 V1504 S1505 A1506 L1509 E1517 E1518 D1519 A1520 L1521 S1522 D1525 K1526 M1531 D1535 L1547 G1553
L1561 E1564 E1567 F1568 I1571 K1581 L1587 V1588 M1589 D1590 V1591 L1592 N1593 I1594 Q1595 R1599 R1603 E1610 I1611 Q1612 K1613 A1614 L1615 Y1618 R1621 S1624 E1635 F1658 V1661 I1665 S1671 E1683 T1693 L1716 K1729 A1730 T1731 S1732 I1756
S1768 MET GLY GLY GLY GLY ASP A1775 L1782 L1789 S1795 Q1800 P1801 P1802 L1803 R1804 R1805 R1819 R1823 I1826 F1836 L1839 S1840 R1843 F1844 K1849 V1853 Q1856 I1859 Q1860 K1865 Y1868 L1879 V1880 L1884 R1887 M1892 T1893 Q1894
R1899 G1902 S1903 G1906 K1912 T1913 E1914 V1927 N1931 C1932 D1933 D1937 F1938 Q1939 R1943 I1944 F1945 V1946 W1954 F1960 L1963 I1978 L1982 N1987 PRO ASN TYR ASP LYS THR SER ALA P1996 C1999 E2000 L2001 K2004 Q2005 V2006 F2015 G2024
K2034 L2035 F2036 M2041 S2056 L2065 I2069 Q2079 L2080 H2085 R2091 K2112 R2113 E2114 LYS GLU GLU ARG GLY GLU ALA VAL ASP GLU GLY GLU ILE A2128 L2137 D2153 L2178 G2194 V2204 E2205 K2206 Y2211 Q2212 I2213 L2220 V2223 S2231 L2237
L2238 K2239 E2242 R2243 L2244 E2248 I2253 A2258 N2271 T2272 R2273 D2289 Q2299 V2302 D2306 V2307 D2308 W2311 N2314 L2315 N2316 N2329 V2339 M2342 F2343 E2344 V2345 A2351 T2352 L2353 R2358 M2361 V2362 W2363 L2382 P2386 E2389 GLY GLU ASP
GLU ALA GLN ARG ARG LYS GLY LYS GLU ASP GLU GLY GLU GLU ALA A2409 L2413 Q2414 I2415 Q2416 R2417 D2418 T2421 Q2442 D2448 L2449 R2453 N2468 V2469 A2470 Q2471 D2478 M2481 E2484 R2488 Y2496 S2503 G2504 D2505 L2514 Y2517 I2518 R2519 R2520


T2523 V2524 P2525 L2526 P2527 T2528 A2529 P2530 N2531 D2536 I2541 E2544 W2545 A2550 K2551 V2552 P2553 Q2554 I2555 E2556 H2560 K2561 V2562 A2563 A2564 P2565 D2566 V2567 V2568 V2569 P2570 D2573 R2576 H2577 E2578 L2581 L2585 L2593 C2594 G2595 P2596 K2601 F2606 S2607 A2608 L2609 R2610 A2611
L2612 P2613 D2614 V2617 E2640 P2645 N2646 V2653 V2660 D2670 M2671 D2672 K2673 S2681 F2682 I2683 R2684 Q2685 M2686 V2687 E2688 D2697 L2703 R2726 F2727 L2728 R2729 H2730 V2731 G2740 P2741 A2742 S2743 L2744 Y2748 G2749 T2750 R2753 L2756 R2757 L2758 I2759 P2760 S2761 L2762 R2763
A2766 E2767 P2768 L2769 T2770 A2771 A2772 M2773 V2774 E2775 F2776 Y2777 T2778 Q2781 E2782 Q2786 H2791 S2795 R2804 F2807 E2808 A2809 L2810 R2811 P2812 L2813 E2814 T2815 L2816 P2817 V2818 E2819 Q2834 D2835 R2836 L2837 D2840 E2841 E2842 R2843 I2850 L2855 K2856 N2860 I2861 D2862 R2863
I2871 D2880 D2885 R2890 R2896 E2903 F2912 N2913 L2916 I2922 F2926 R2927 Q2928 L2933 L2934 V2950 M2953 L2956 K2966 Y2967 T2968 G2969 E2970 R2977 R2982 N2987 E2988 K2989 I2990 D2995 E2996 S2997 L3000 D3001 S3002 G3003 F3004 L3005 N3009
L3020 D3024 L3042 M3043 L3044 K3052 N3061 V3065 F3066 T3067 M3068 S3071 S3072 E3073 G3074 L3075 K3076 D3077 R3078 A3079 A3080 T3081 S3082 P3083 A3084 L3085 F3086 N3087 D3096 W3097 S3098 F3109 T3110 S3111 E3116 I3121 D3124 K3132 L3133 P3134 Q3135 P3136 R3140 V3150 H3155
R3164 G3165 G3166 R3174 I3180 E3189 L3194 R3206 E3217 R3220 R3223 I3224 K3225 S3226 Q3227 E3228 L3229 E3230 V3231 K3232 N3233 A3234 A3235 A3236 N3237 D3238 K3239 L3240 LYS LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS LYS VAL MET SER GLN GLU ILE GLN GLU GLN
LEU HIS LYS GLN GLN GLU VAL ILE ALA ASP LYS GLN MET SER VAL LYS GLU ASP LEU ASP LYS VAL GLU PRO ALA VAL ILE GLU ALA GLN ASN ALA 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 ARG SER ILE ILE MET ARG GLU ASN PHE ILE PRO THR ILE ILE VAL ASN PHE SER ALA GLU GLU LYS ILE SER ASP ALA ILE ARG GLU LYS MET LYS LYS ASN TYR MET SER ASN PRO SER TYR ASN TYR GLU ILE VAL ASN
ARG ALA SER LEU ALA CYS GLY PRO MET VAL LYS TRP ALA ILE ALA GLN LEU ASN TYR ALA ASP MET LEU LYS ARG VAL GLU PRO LEU ARG ASN GLU LEU GLN LYS LEU GLU ASP ASP ALA LYS ASP ASN GLN GLN LYS ALA ASN GLU VAL GLU GLN MET ILE ARG ASP LEU GLU ALA SER
ILE ALA ARG TYR LYS GLU E3450 Y3451 A3452 V3453 L3454 I3455 S3456 E3457 A3458 Q3459 A3460 I3461 K3462 A3463 D3464 L3465 A3466 S3475 L3479 K3480 S3481 A3484 E3487 N3498 T3502 I3503 F3520 M3524 W3532 D3546 I3547 S3554 R3559 D3570 R3582 R3585 S3593 G3594
R3611 D3617 E3624 R3628 Q3636 E3639 P3643 G3658 G3665 D3666 Q3667 D3668 S3680 T3685 V3686 E3687 Q3709 C3712 E3715 D3723 V3724 D3725 D3730 L3740 R3741 L3745 L3749 L3750 Q3751 K3757 G3758 R3759 I3760 L3761 D3762 I3766 I3767 T3768
L3773 E3776 R3782 M3791 E3795 S3805 M3815 F3823 L3824 Y3825 N3845 L3846 LYS GLY V3849 T3850 R3855 K3861 F3868 A3872 M3875 H3880 I3881 T3882 F3883 A3884 M3885 L3886 L3887 A3888 K3891 T3895 VAL G3897 S3917 A3918 P3922 A3932 D3946
W3974 SER GLU GLU T3978 R3997 V4009 N4012 I4030 E4034 P4037 Q4065 I4071 E4075 G4076 F4077 N4078 D4081 K4082 K4089 V4099 L4106 S4115 P4118 M4128 K4133 R4140 P4150 K4154 R4159 T4160 S4172 R4176 E4192 S4210
D4211 L4212 T4226 A4227 K4228 N4232 P4239 L4246 G4253 F4268 V4288 D4289 G4290 H4291 E4310 T4315 P4318 L4321 N4325 N4326 M4339 K4342 M4346 Q4347 M4348 L4349 E4350 ASP GLU ASP ASP LEU ALA TYR ALA GLU THR GLU LYS LYS THR ARG THR ASP SER



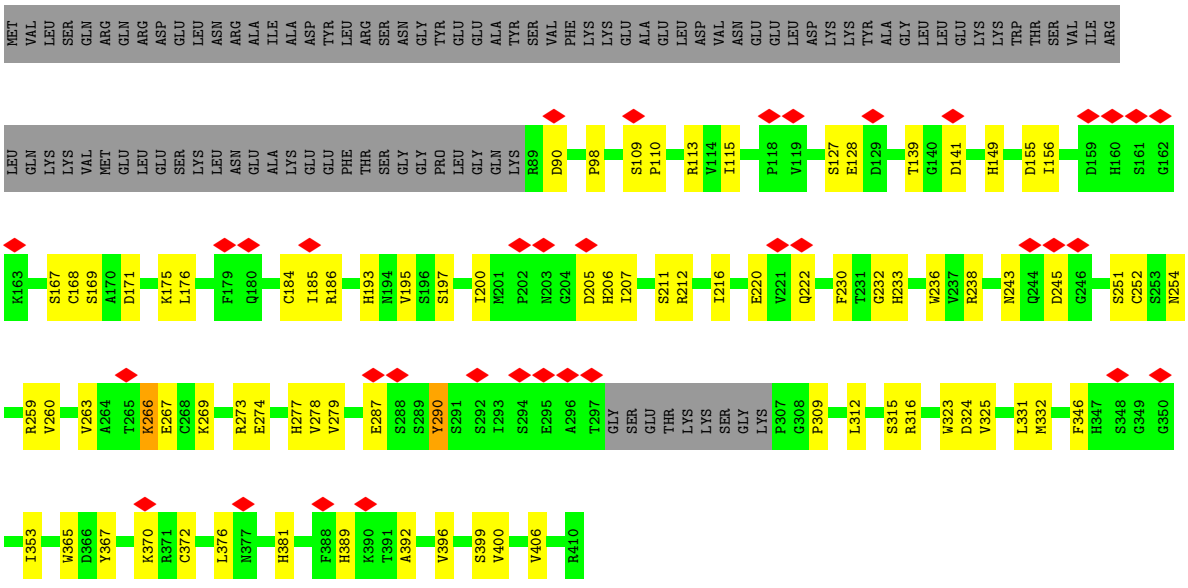
• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain B:



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90594	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	296.52002, 296.52002, 296.52002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/23286	0.57	12/31602 (0.0%)
2	B	0.27	0/2560	0.62	2/3470 (0.1%)
2	C	0.29	0/2560	0.64	2/3470 (0.1%)
All	All	0.28	0/28406	0.58	16/38542 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3643	PRO	CA-N-CD	-11.84	94.93	111.50
2	C	90	ASP	CB-CG-OD2	8.70	126.13	118.30
2	C	205	ASP	CB-CG-OD2	8.39	125.85	118.30
1	A	2729	ARG	CG-CD-NE	7.06	126.62	111.80
1	A	2671	MET	CA-CB-CG	6.87	124.98	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1963	LEU	Peptide

5.2 Too-close contacts (i)

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	22814	0	22627	222	0
2	B	2494	0	2419	37	0
2	C	2494	0	2419	47	0
3	A	81	0	36	3	0
4	A	2	0	0	0	0
5	A	31	0	12	1	0
All	All	27916	0	27513	302	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 302 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:2316:ASN:HB2	1:A:2358:ARG:NH2	1.92	0.83
1:A:2231:SER:OG	5:A:4803:ATP:O2B	1.97	0.81
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.01	0.77
1:A:2220:LEU:HB2	1:A:2342:MET:HG3	1.71	0.71
1:A:4384:ALA:O	1:A:4388:LEU:HB2	1.93	0.68

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	2864/4646 (62%)	2763 (96%)	100 (4%)	1 (0%)	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	309/410 (75%)	294 (95%)	15 (5%)	0	100	100
2	C	309/410 (75%)	292 (94%)	17 (6%)	0	100	100
All	All	3482/5466 (64%)	3349 (96%)	132 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2871	ILE

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	2459/4125 (60%)	2415 (98%)	44 (2%)	59	77
2	B	280/364 (77%)	271 (97%)	9 (3%)	39	65
2	C	280/364 (77%)	274 (98%)	6 (2%)	53	74
All	All	3019/4853 (62%)	2960 (98%)	59 (2%)	57	75

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3206	ARG
2	C	290	TYR
1	A	3997	ARG
2	C	267	GLU
2	B	225	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2471	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
3	ADP	A	4806	-	24,29,29	0.95	1 (4%)	29,45,45	1.57	4 (13%)
3	ADP	A	4805	-	24,29,29	0.93	1 (4%)	29,45,45	1.52	4 (13%)
3	ADP	A	4801	4	24,29,29	0.99	1 (4%)	29,45,45	1.44	6 (20%)
5	ATP	A	4803	4	26,33,33	0.61	0	31,52,52	0.76	1 (3%)

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	A	4806	-	-	2/12/32/32	0/3/3/3
3	ADP	A	4805	-	-	1/12/32/32	0/3/3/3
3	ADP	A	4801	4	-	1/12/32/32	0/3/3/3
5	ATP	A	4803	4	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4806	ADP	C5-C4	2.49	1.47	1.40
3	A	4805	ADP	C5-C4	2.46	1.47	1.40
3	A	4801	ADP	C5-C4	2.45	1.47	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4806	ADP	PA-O3A-PB	-3.96	119.23	132.83
3	A	4806	ADP	C3'-C2'-C1'	3.76	106.64	100.98
3	A	4805	ADP	C3'-C2'-C1'	3.65	106.48	100.98
3	A	4805	ADP	N3-C2-N1	-3.55	123.13	128.68
3	A	4801	ADP	PA-O3A-PB	-3.46	120.97	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4806	ADP	O4'-C4'-C5'-O5'
3	A	4806	ADP	C3'-C4'-C5'-O5'
3	A	4801	ADP	O4'-C4'-C5'-O5'
5	A	4803	ATP	O4'-C4'-C5'-O5'
5	A	4803	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

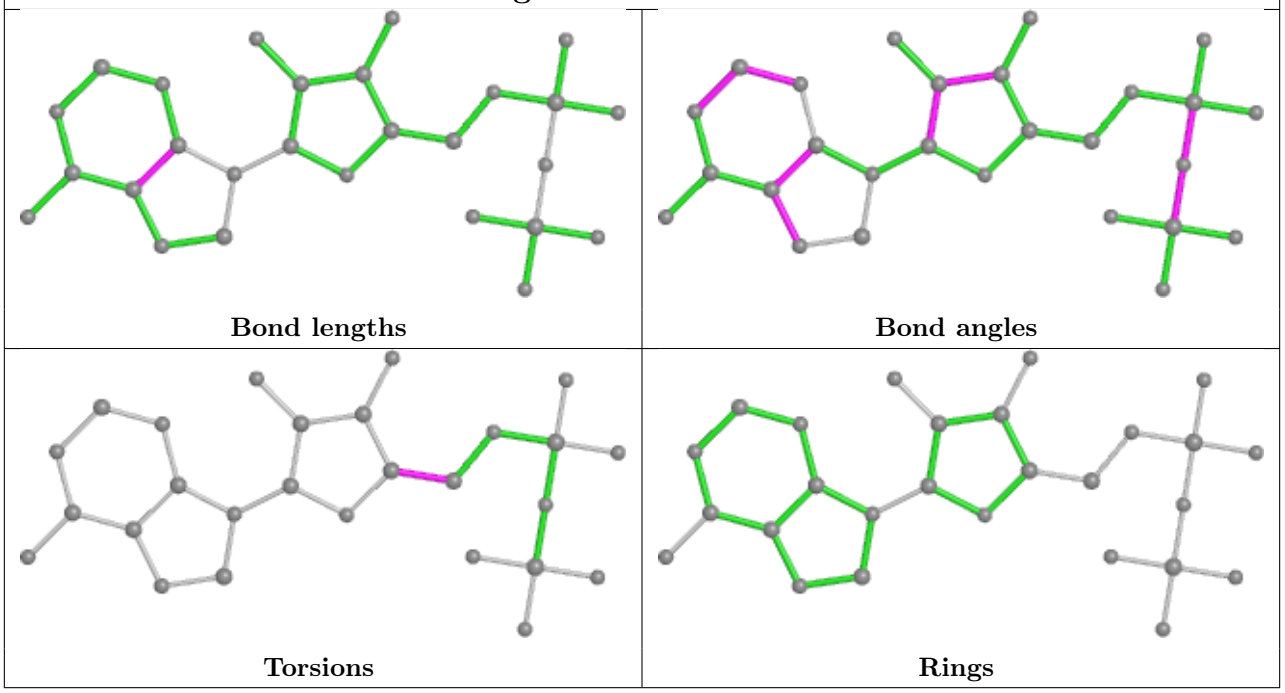
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4806	ADP	1	0
3	A	4801	ADP	2	0
5	A	4803	ATP	1	0

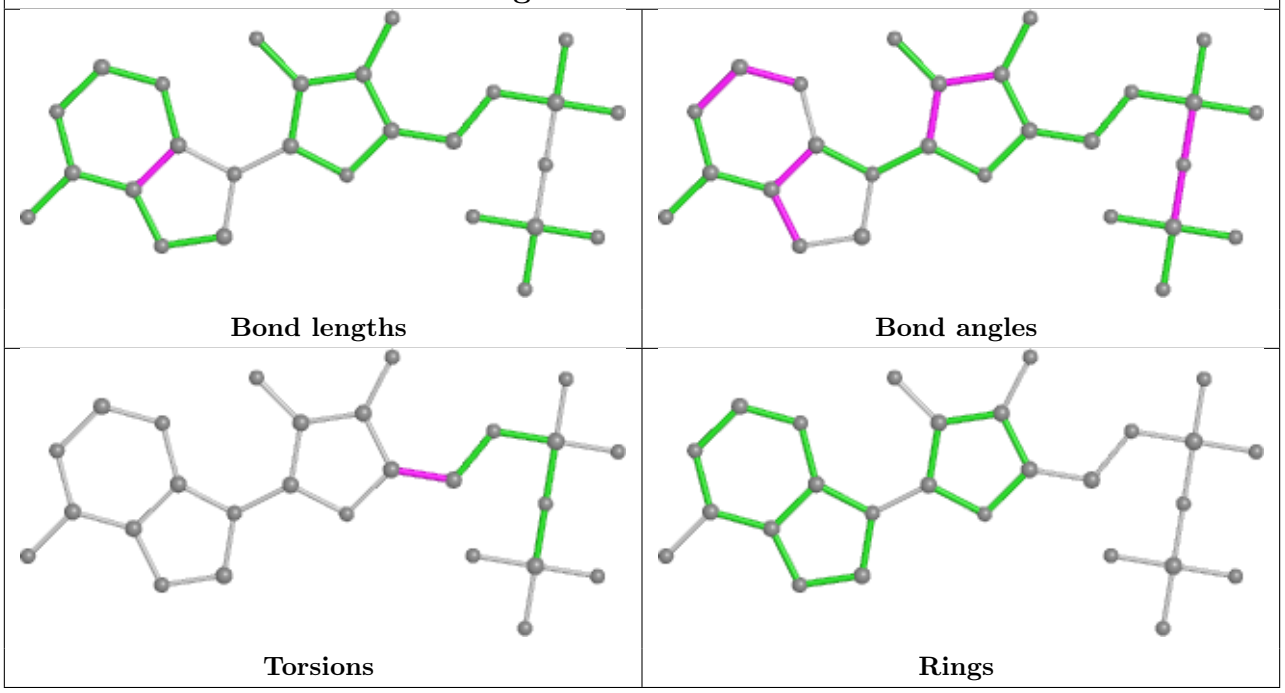
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

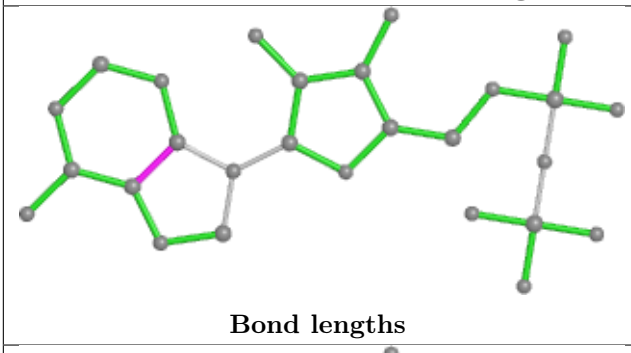
Ligand ADP A 4806



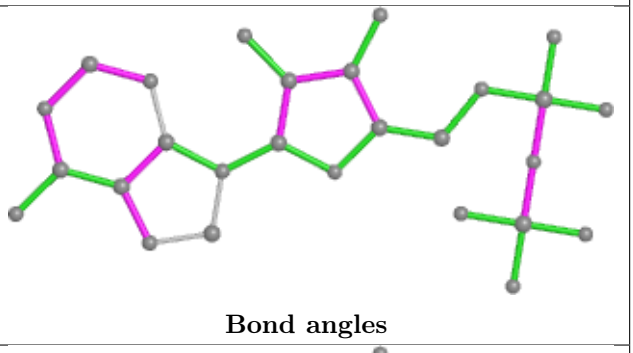
Ligand ADP A 4805



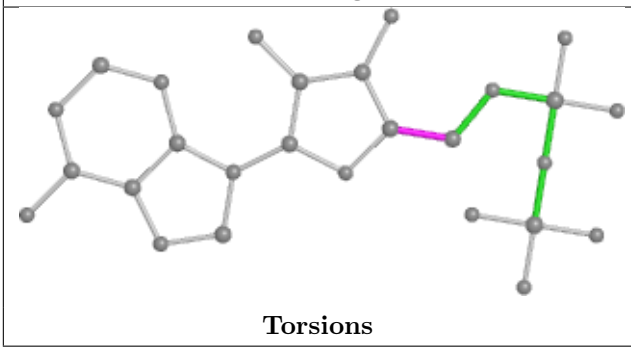
Ligand ADP A 4801



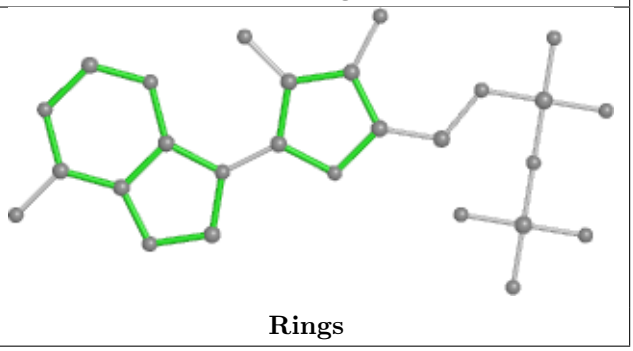
Bond lengths



Bond angles

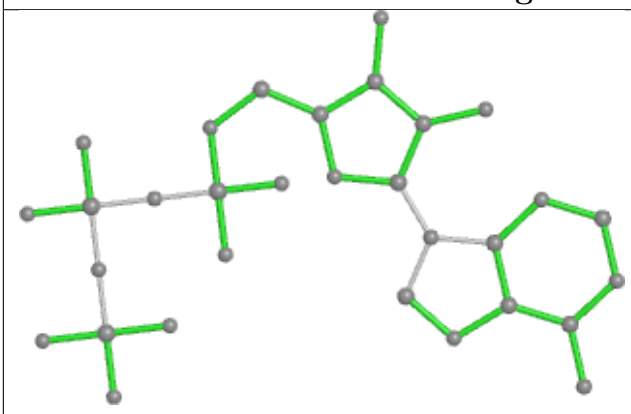


Torsions

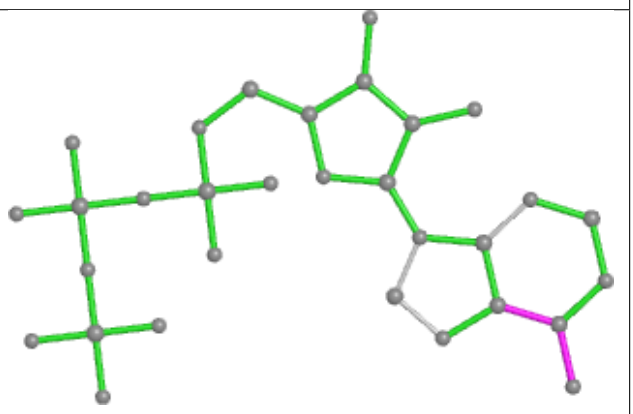


Rings

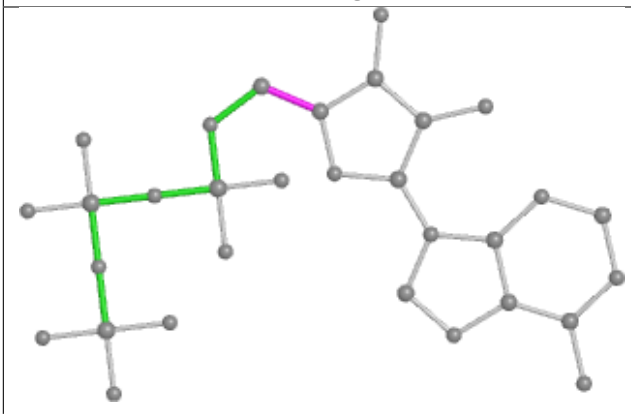
Ligand ATP A 4803



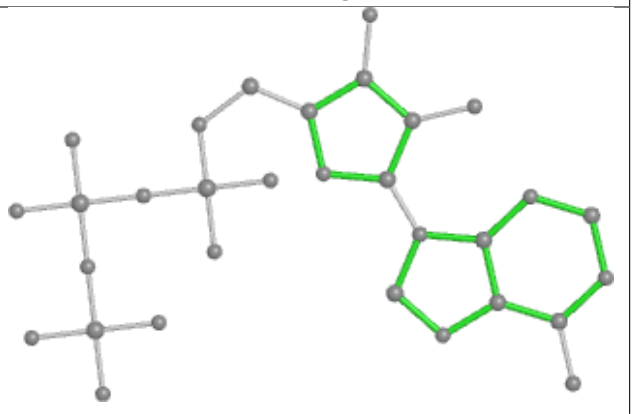
Bond lengths



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.

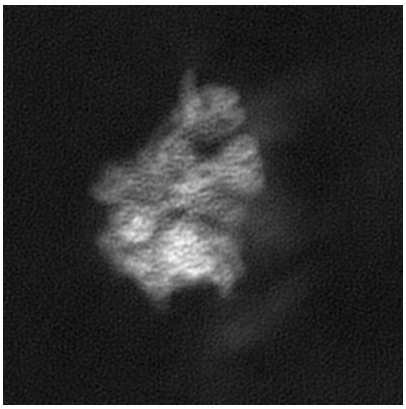
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17828. These allow visual inspection of the internal detail of the map and identification of artifacts.

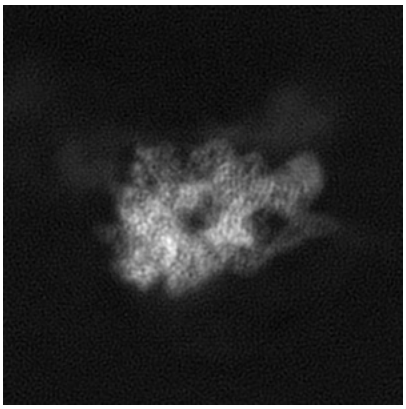
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

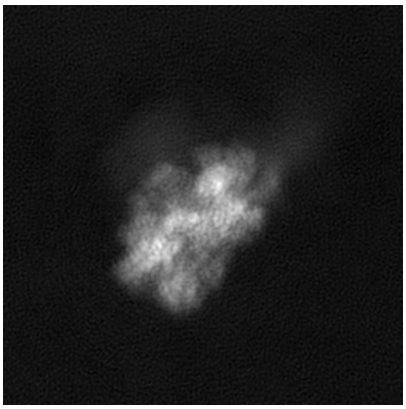
6.1.1 Primary map



X

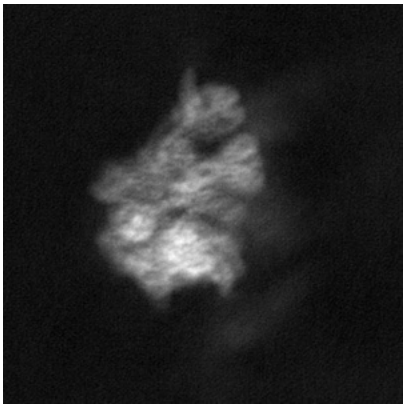


Y

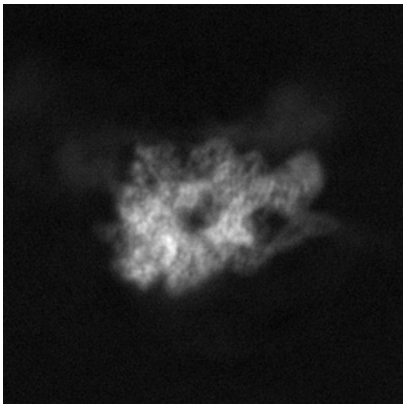


Z

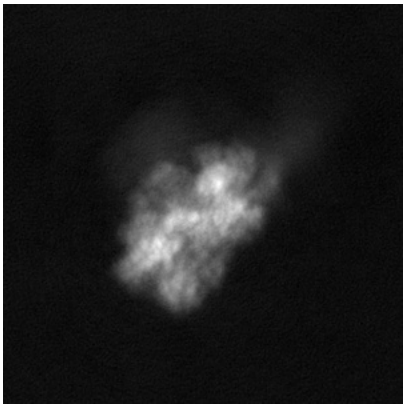
6.1.2 Raw map



X



Y

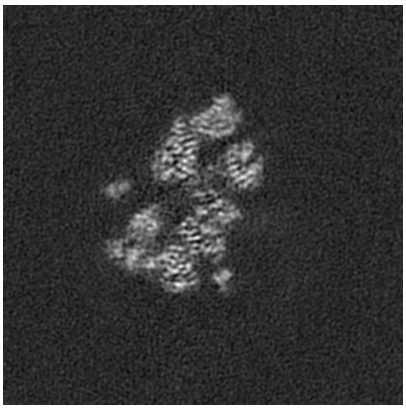


Z

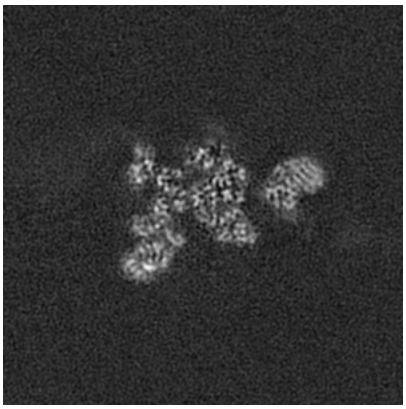
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

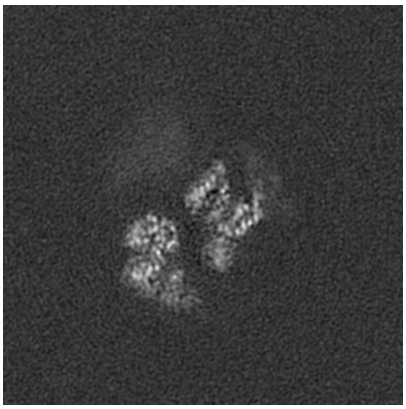
6.2.1 Primary map



X Index: 140

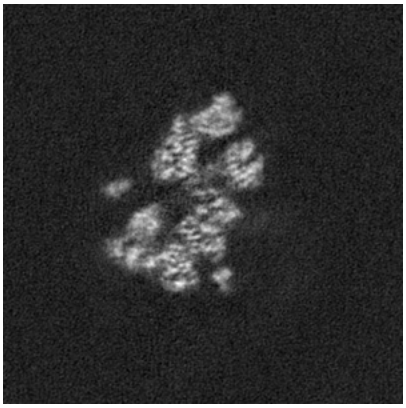


Y Index: 140

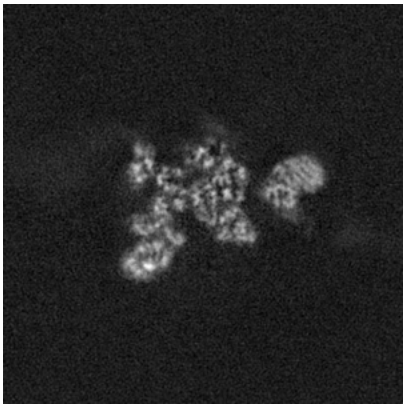


Z Index: 140

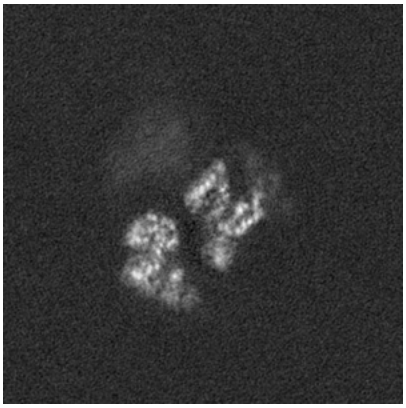
6.2.2 Raw map



X Index: 140



Y Index: 140

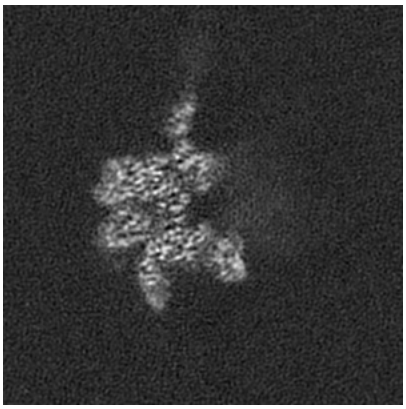


Z Index: 140

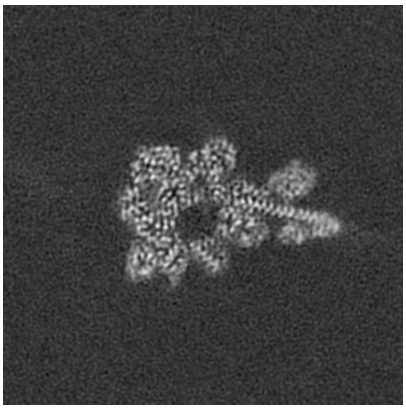
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

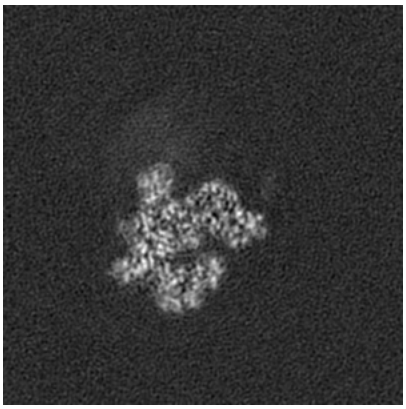
6.3.1 Primary map



X Index: 116

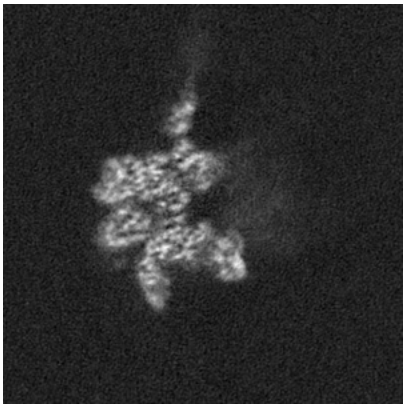


Y Index: 130

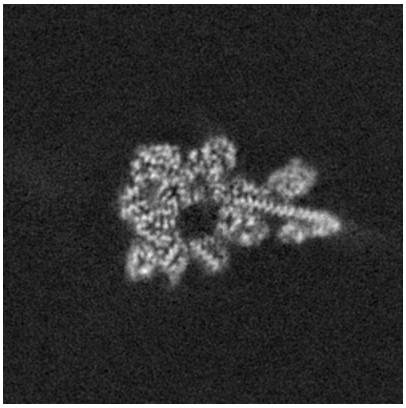


Z Index: 115

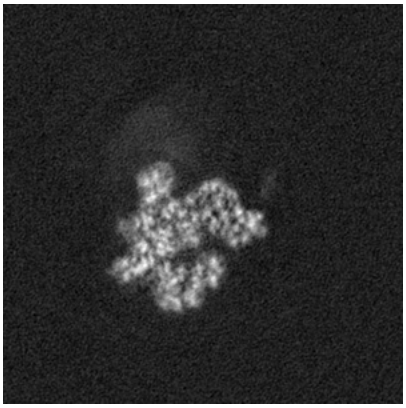
6.3.2 Raw map



X Index: 116



Y Index: 130

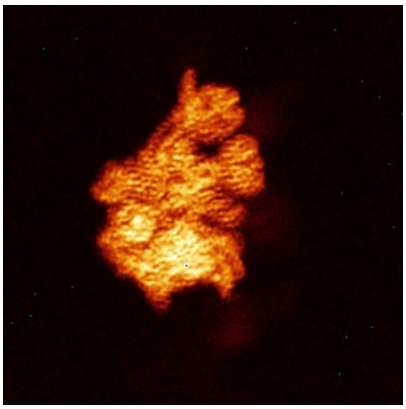


Z Index: 115

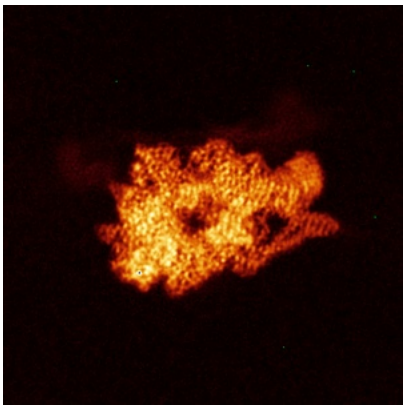
The images above show the largest variance slices of the map in three orthogonal directions.

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

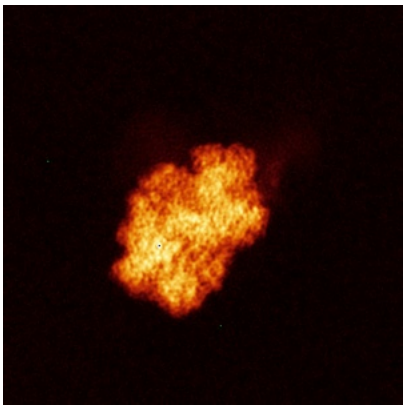
6.4.1 Primary map



X

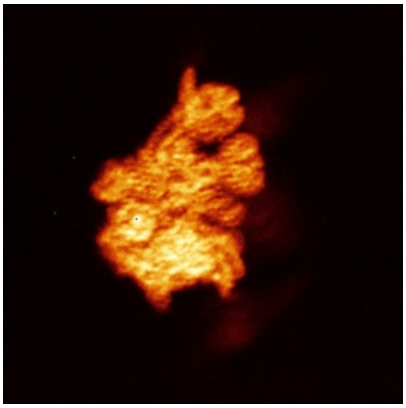


Y

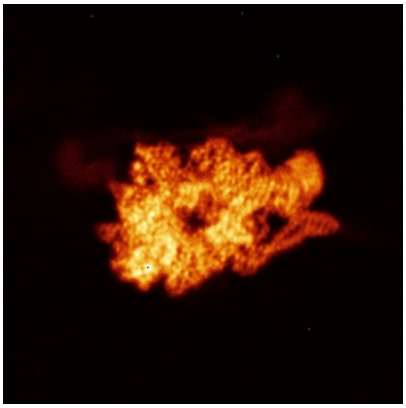


Z

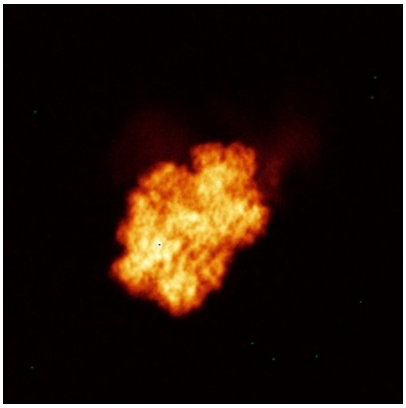
6.4.2 Raw map



X



Y

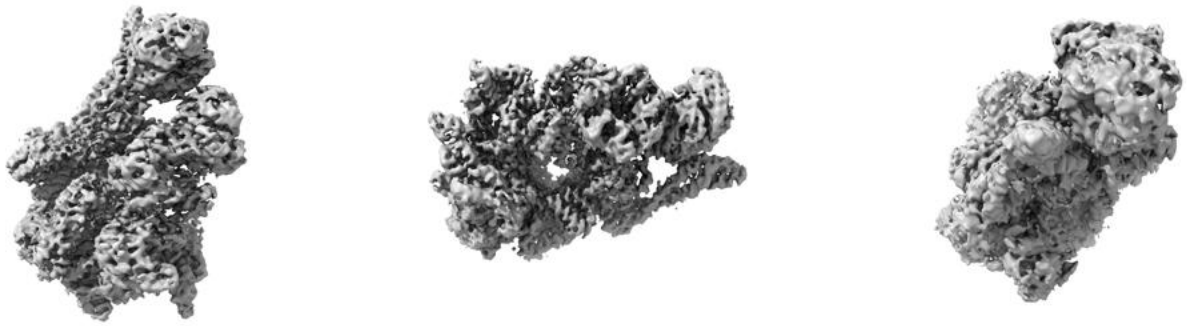


Z

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

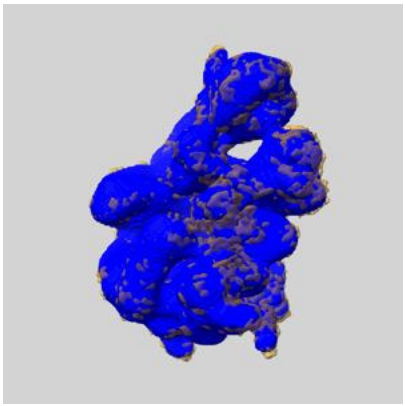
6.6 Mask visualisation (i)

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

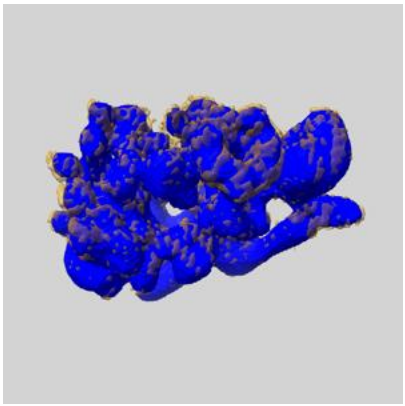
A mask typically either:

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

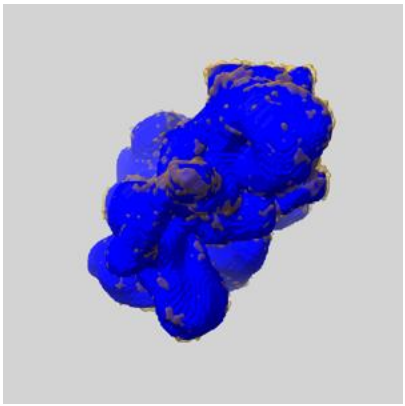
6.6.1 emd_17828_msk_1.map (i)



X



Y

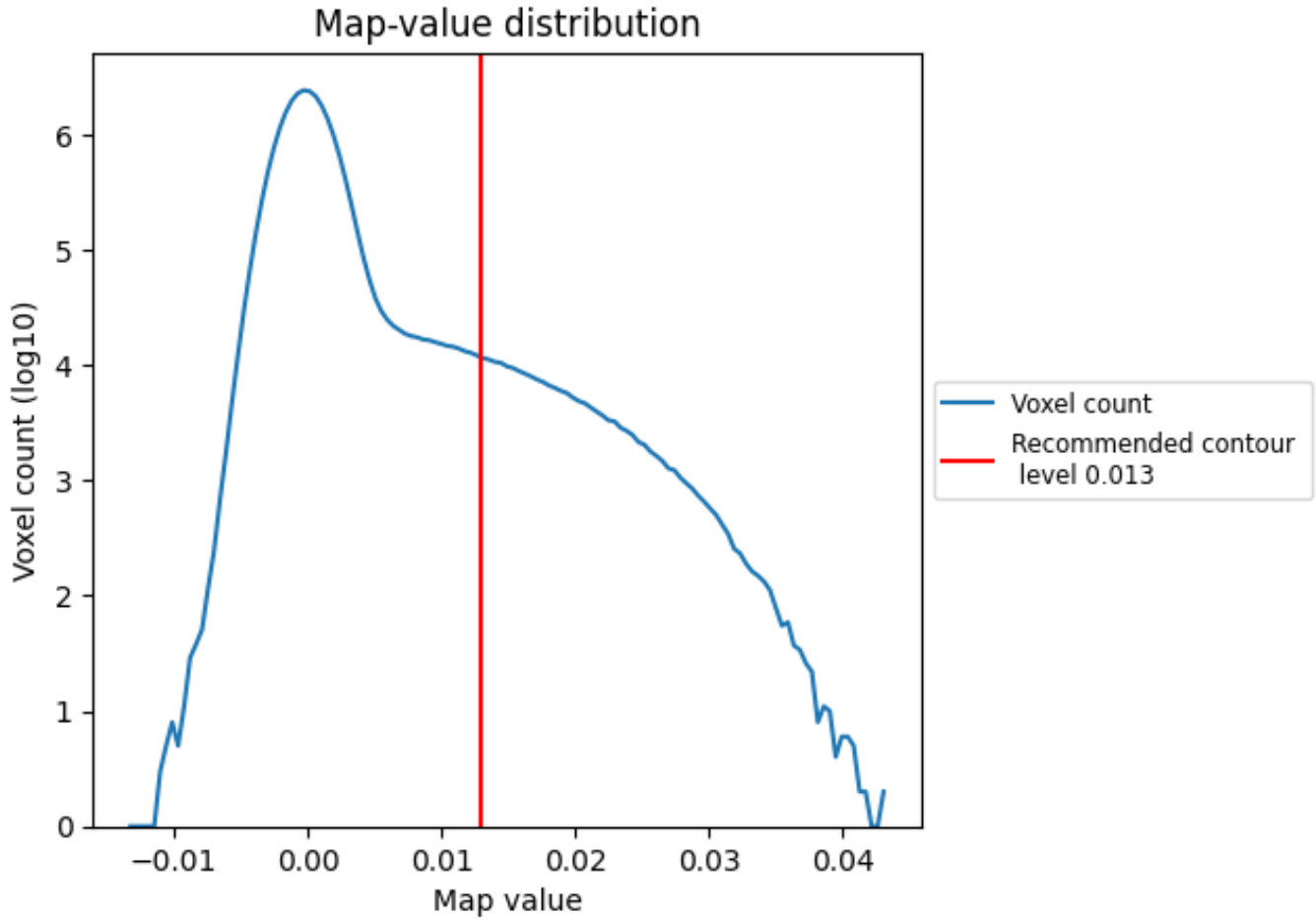


Z

7 Map analysis

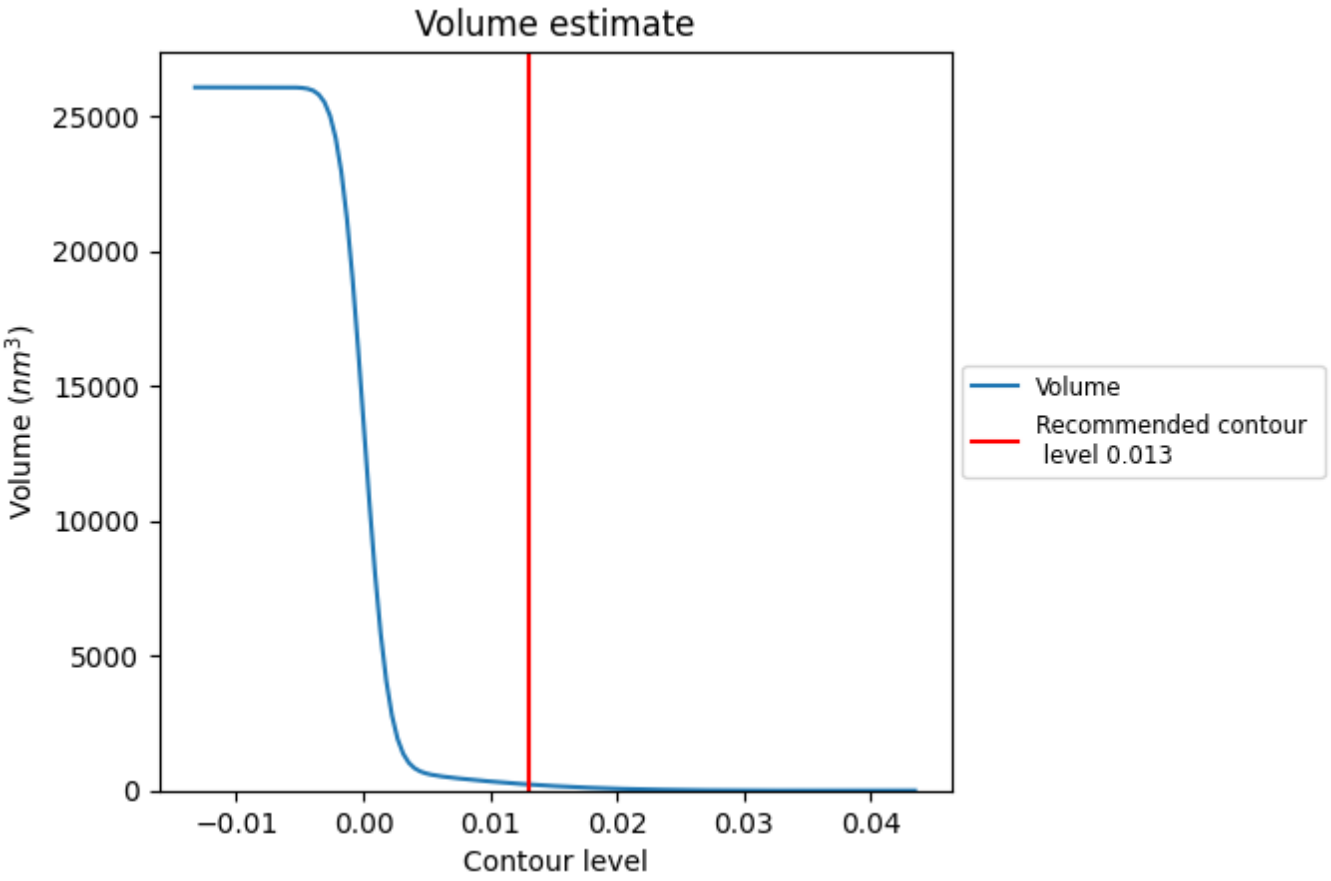
This section contains the results of statistical analysis of the map.

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.

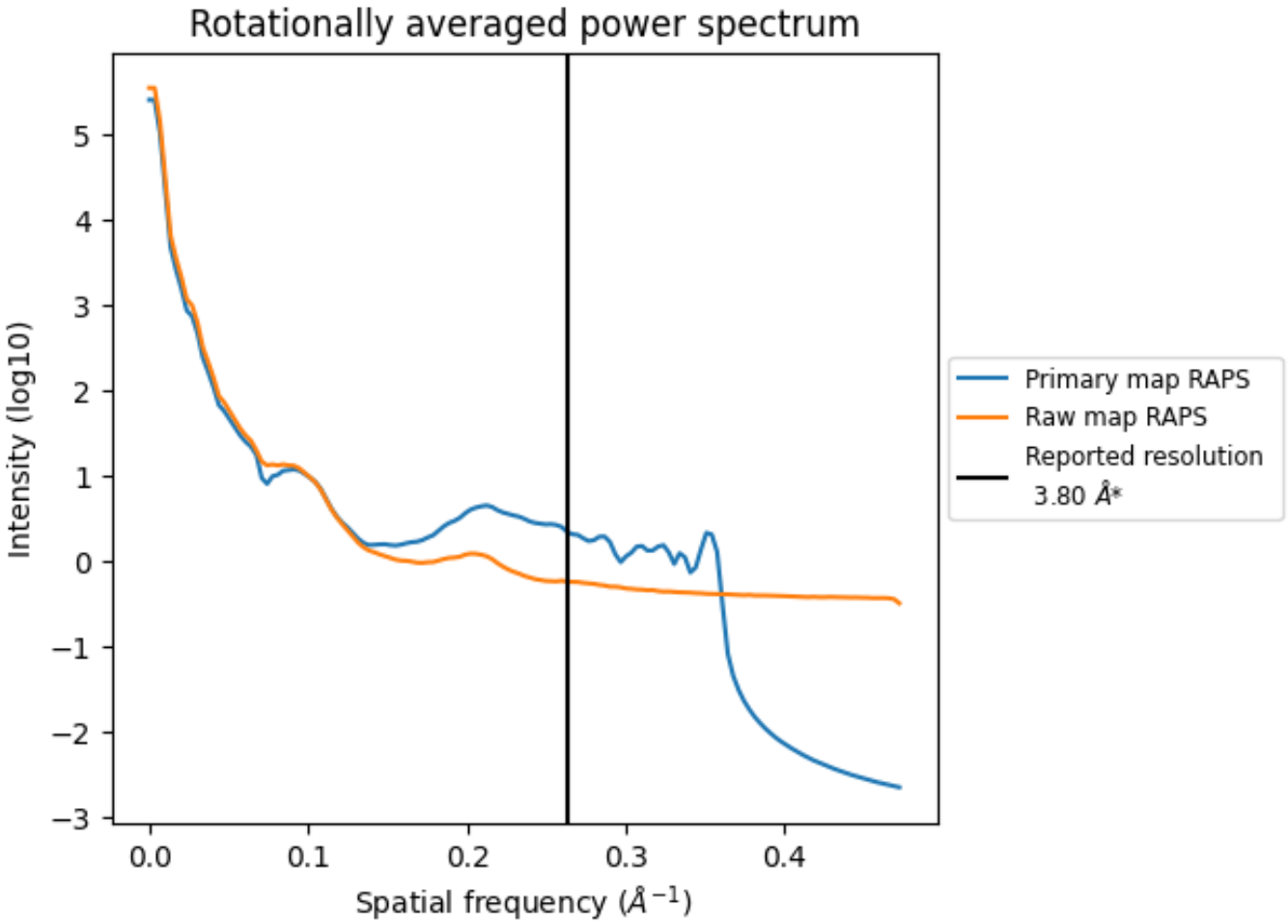
7.2 Volume estimate (i)



The volume at the recommended contour level is 228 nm^3; this corresponds to an approximate mass of 206 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)

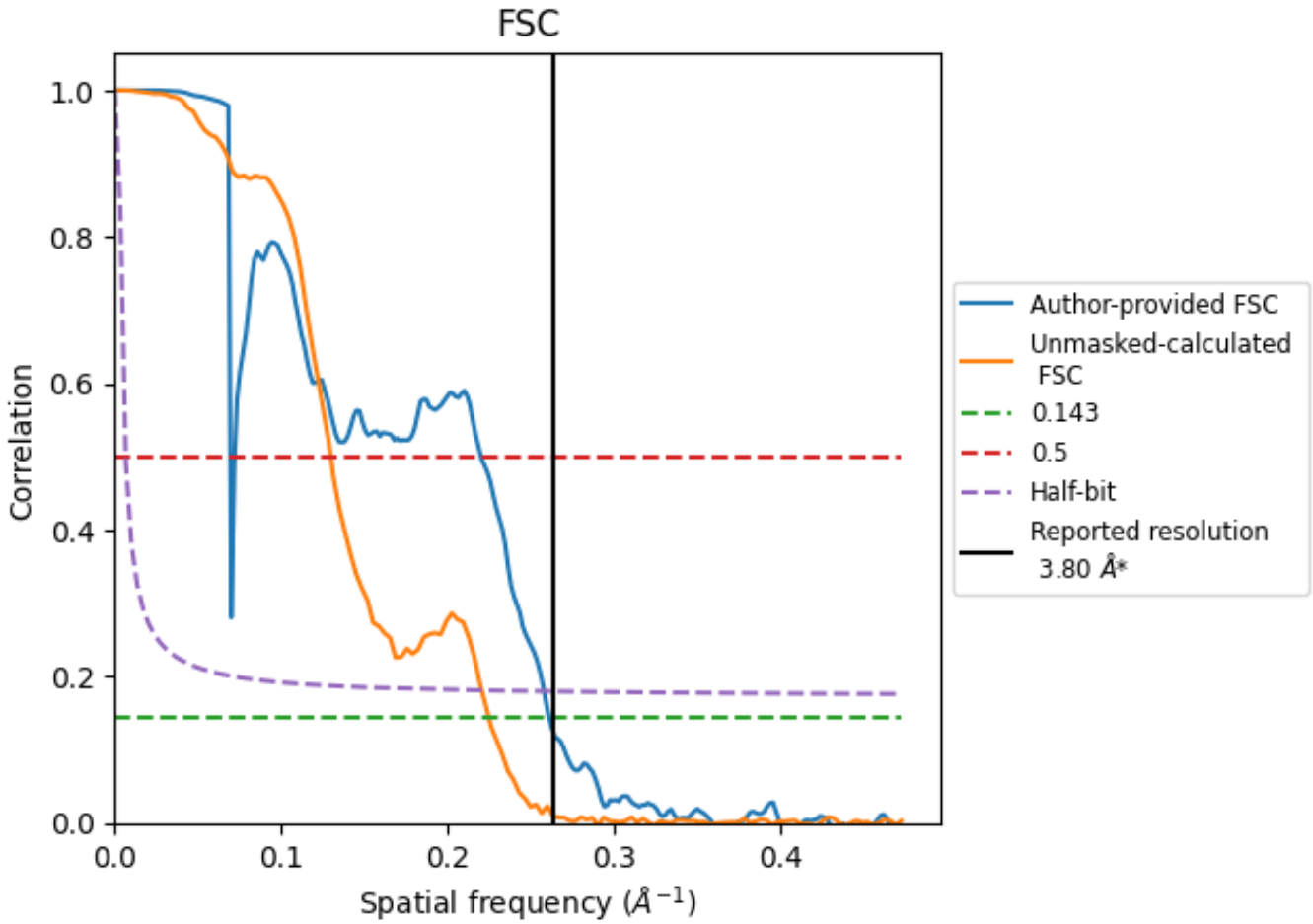


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

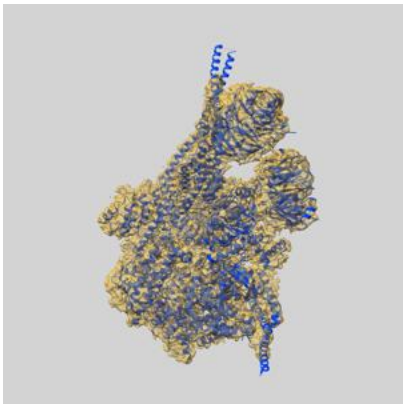
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.84	14.41	3.88
Unmasked-calculated*	4.45	7.72	4.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.45 differs from the reported value 3.8 by more than 10 %

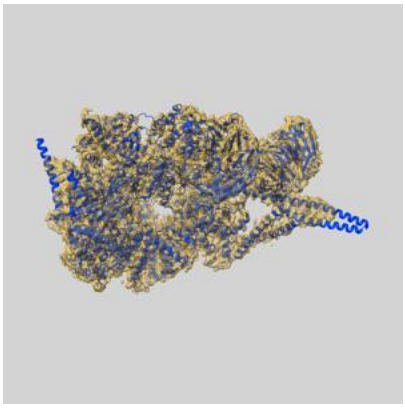
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17828 and PDB model 8PQY. Per-residue inclusion information can be found in section 3 on page 6.

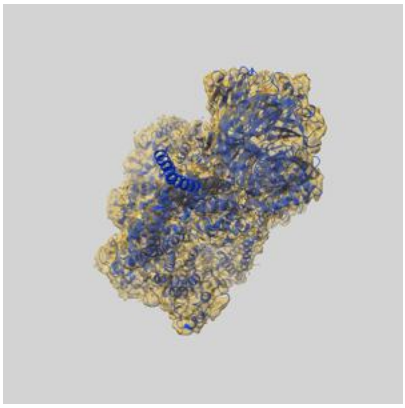
9.1 Map-model overlay



X



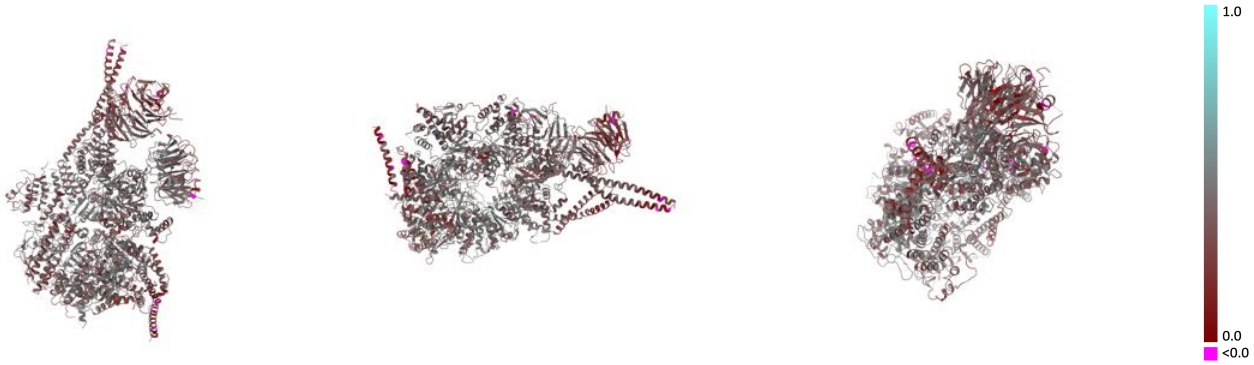
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

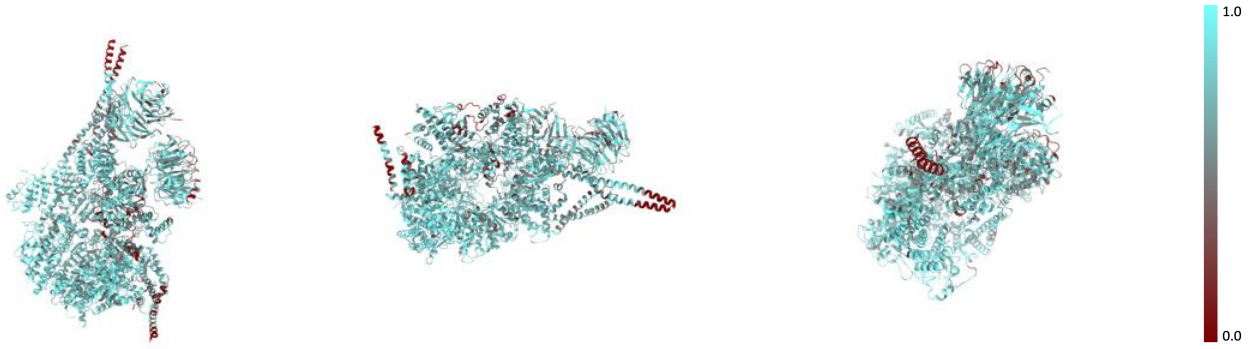
9.2 Q-score mapped to coordinate model



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.

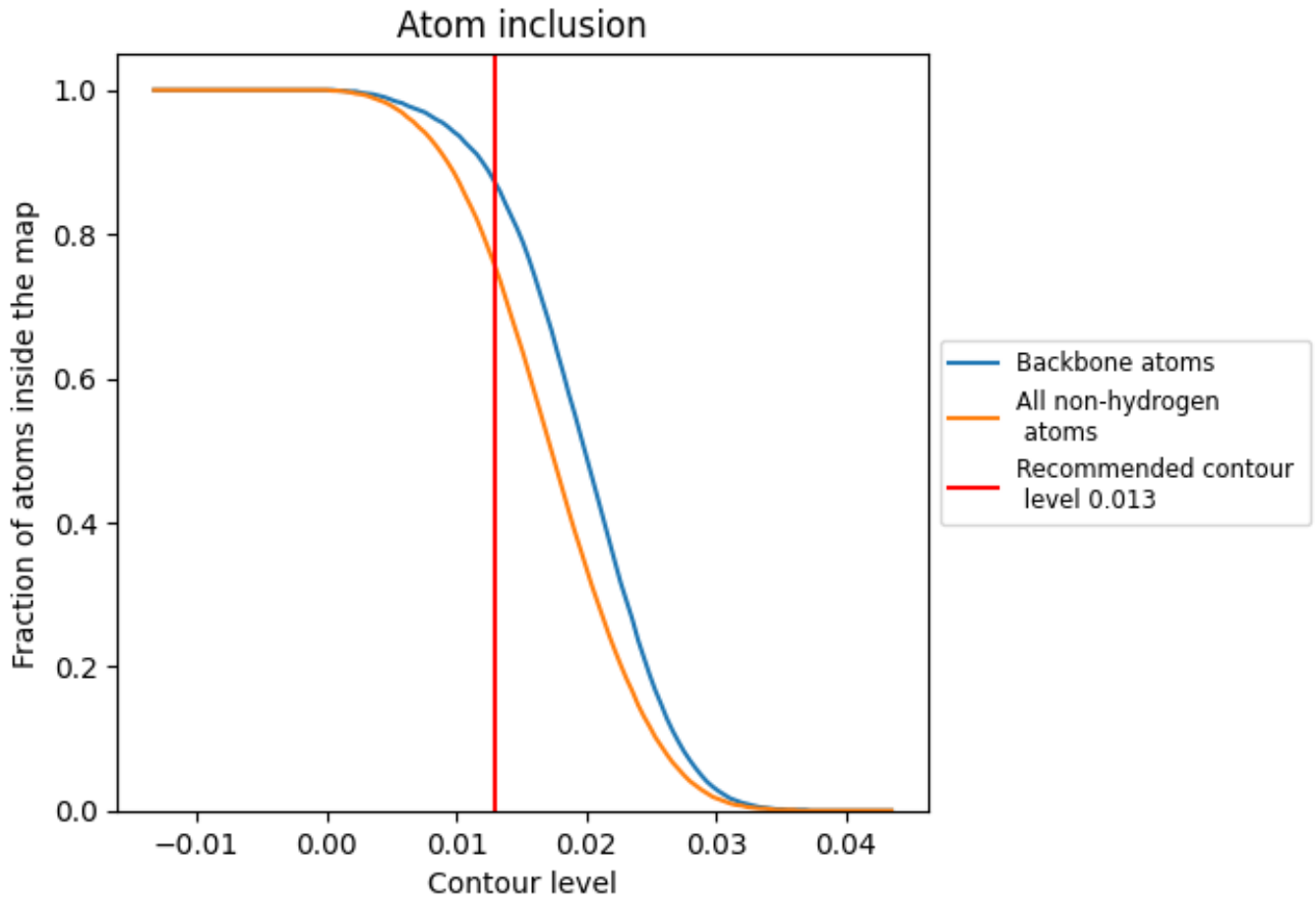
9.3 Atom inclusion mapped to coordinate model



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.3870
A	0.7700	0.3970
B	0.7020	0.3010
C	0.6770	0.3810