wwPDB EM Validation Summary Report

Sep 9, 2026 – 09:43 pm BST

PDB ID	:	8PQV / pdb_00008pqv
EMDB ID	:	EMD-17825
Title	:	Cytoplasmic dynein-1 motor domain in post-powerstroke state
Authors	:	Singh, K.; Lau, C.K.; Manigrasso, G.; Gassmann, R.; Carter, A.P.
Deposited on	:	2023-07-12
Resolution	:	4.00 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:

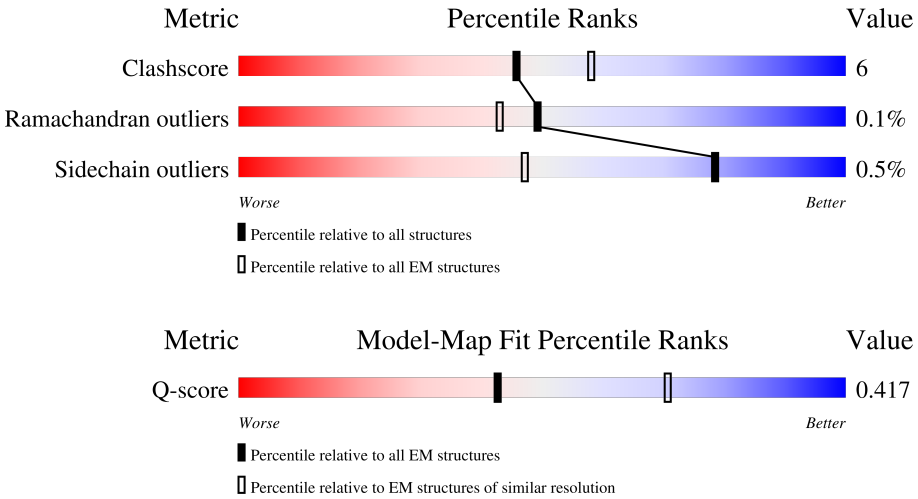
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 4.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	55% 10% 35%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24537 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.

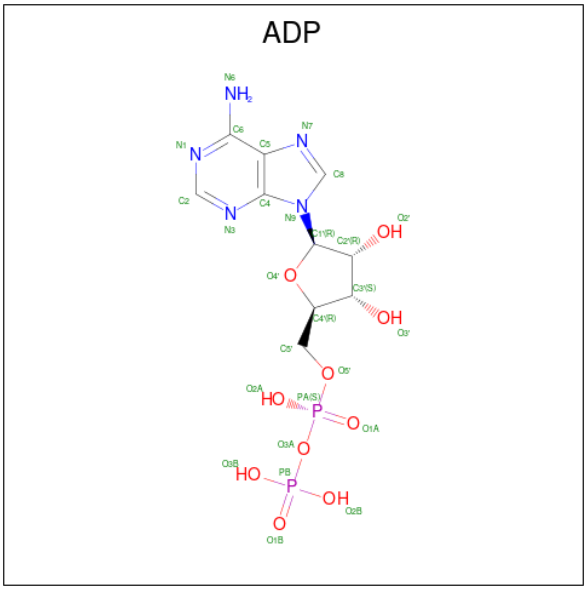
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3032	24417	15554	4210	4531	122	0	0

There are 2 discrepancies between the modelled and reference sequences:

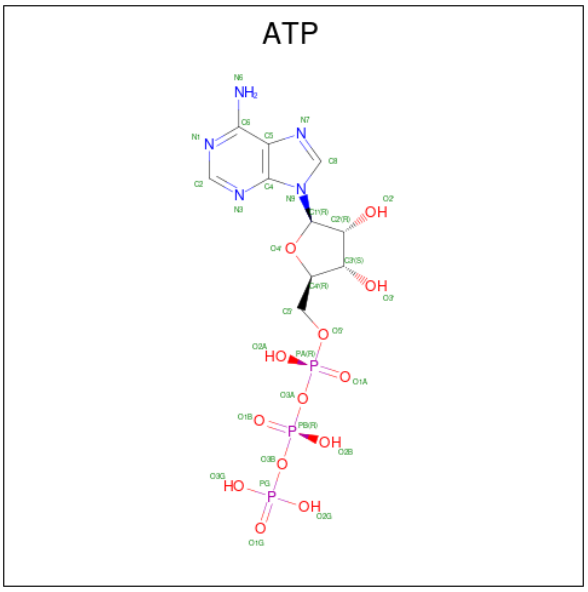
Chain	Residue	Modelled	Actual	Comment	Reference
A	1567	GLU	ARG	engineered mutation	UNP Q14204
A	1610	GLU	LYS	engineered mutation	UNP Q14204

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



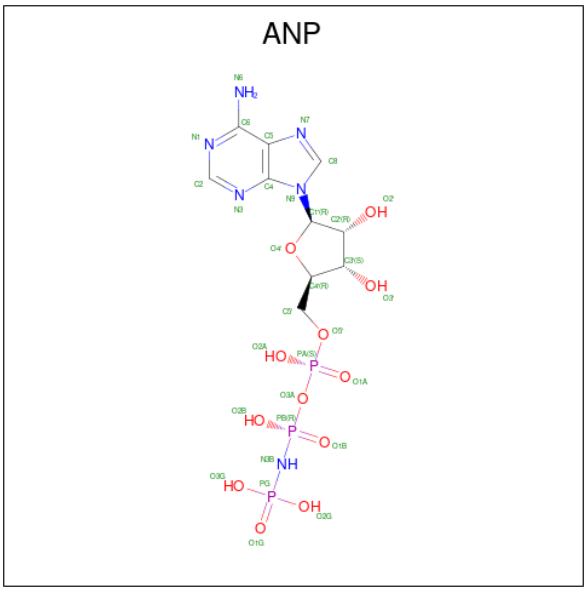
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- 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	
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

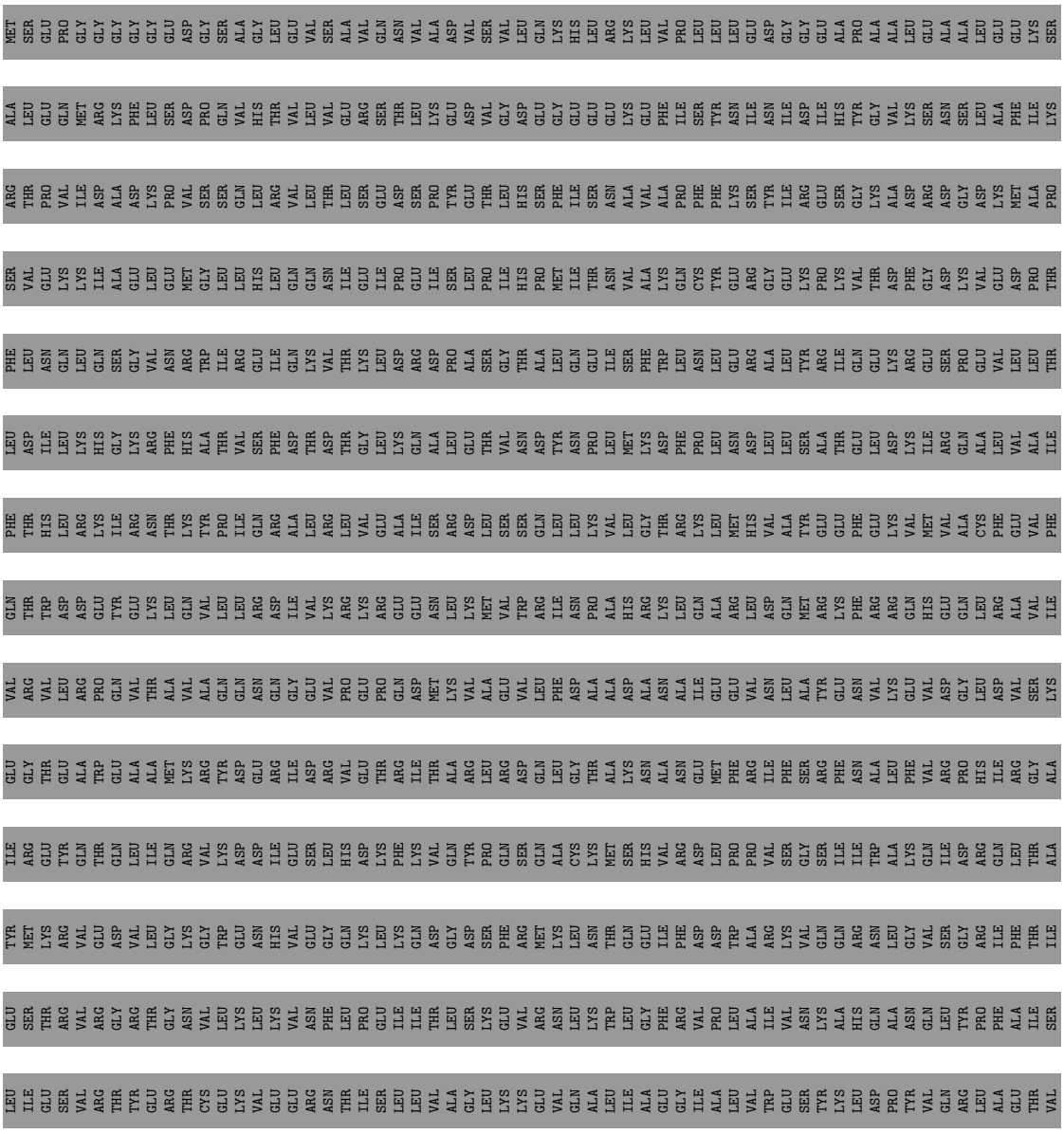
3 Residue-property plots (i)

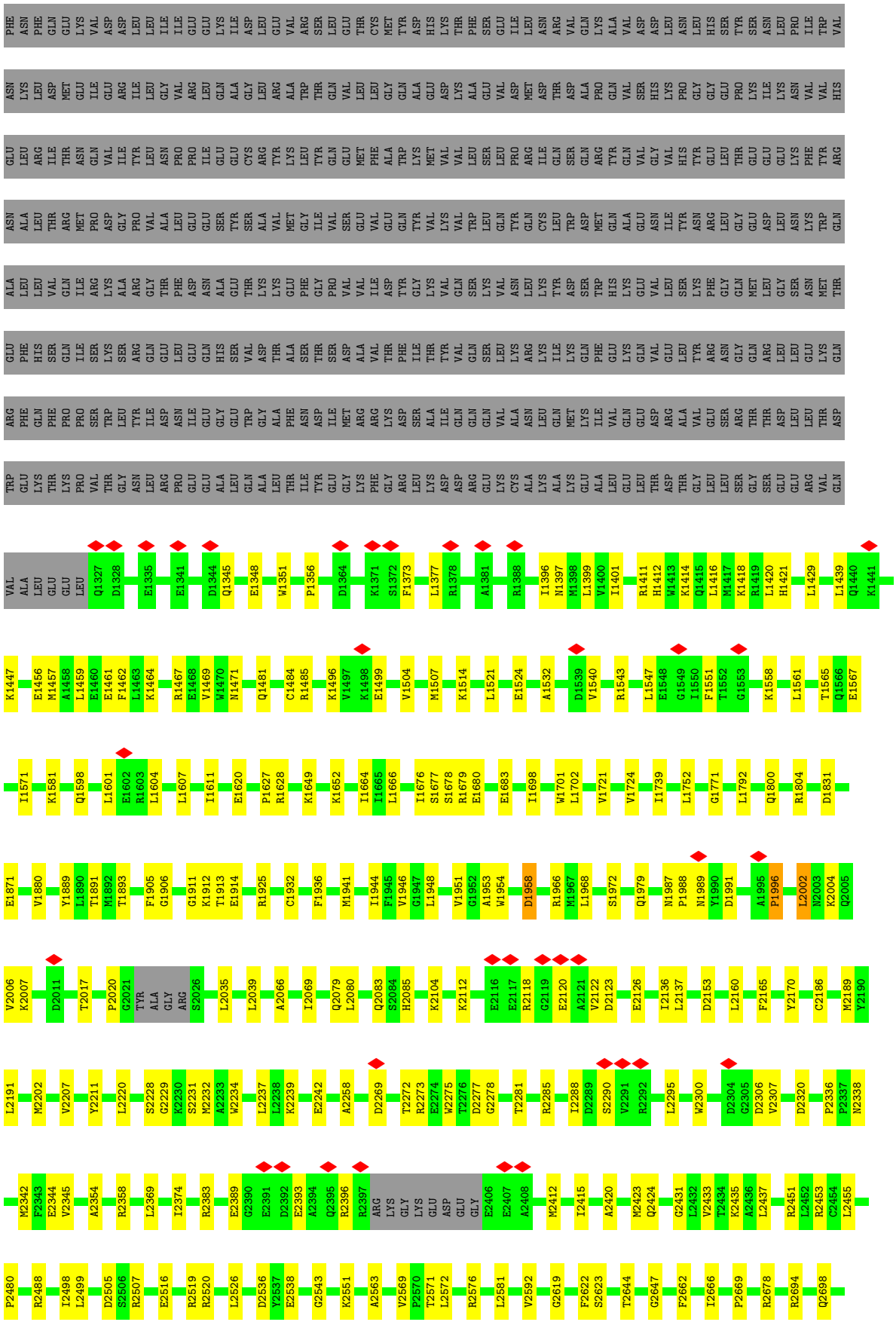
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

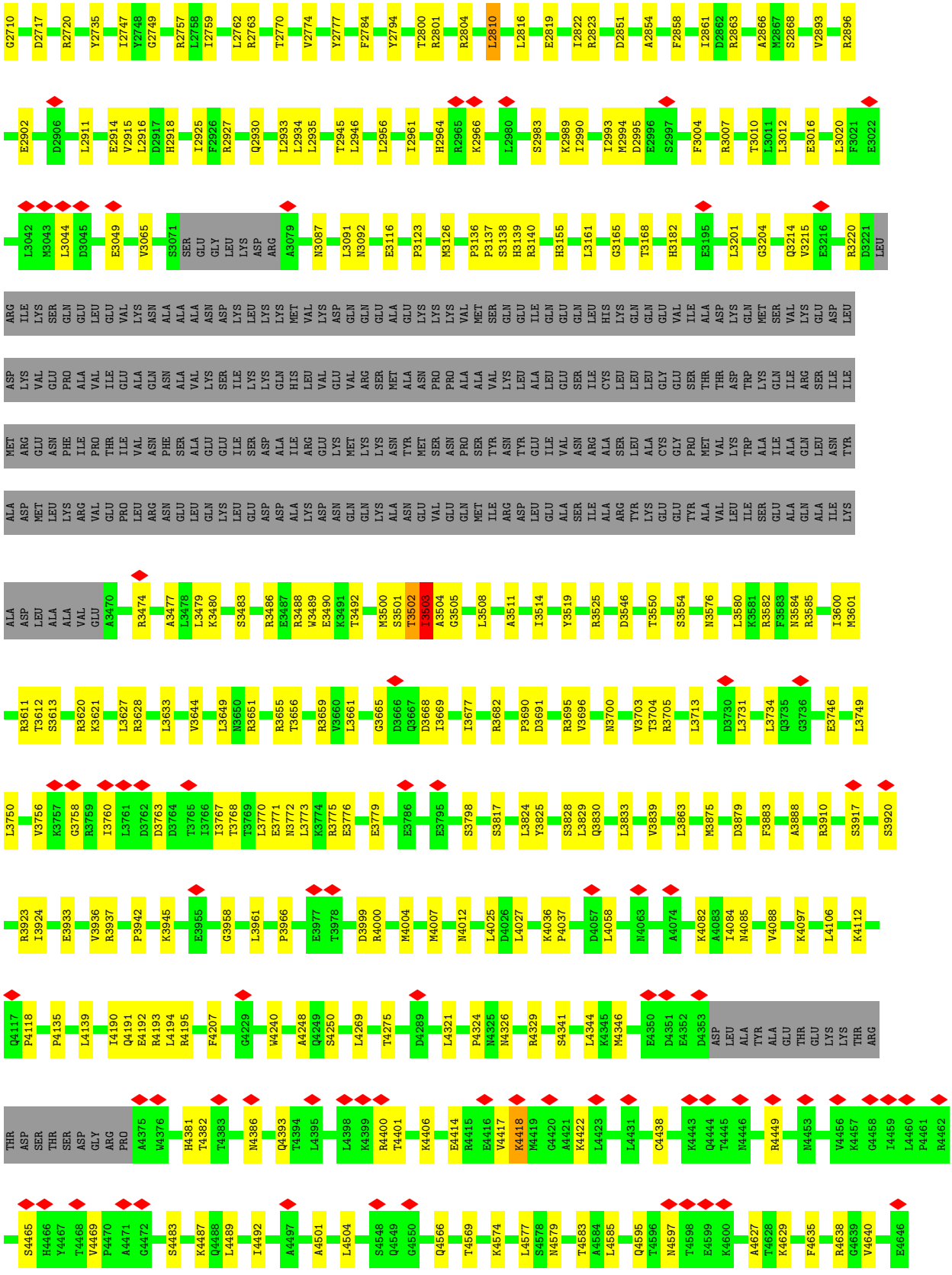
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

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 HIS SER TYR SER ASN LEU PRO ILE VAL
ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ARG LEU GLN ALA GLY LEU ARG 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 GLN ILE GLN SER GLN ARG TYR SER GLY VAL HIS TYR GLU GLU LEU THR GLU GLU GLY LYS PHE TYR ARG
ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER GLU TYR SER ALA VAL MET GLY ILE VAL SER GLU VAL GLY GLN TYR VAL LYS VAL TRP LEU GLN TYR ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU 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 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 ARG GLN GLU LEU GLU GLN HIS SER VAL ASP THR ALA SER THR SER ASP ALA VAL THR PHE ILE THR TYR VAL LYS GLN PHE GLU LYS GLN VAL GLU LEU GLY ARG GLN LEU ASP ILE LYS GLN ARG LYS ILE LYS GLN VAL GLU LEU ARG LEU GLU GLU LYS LYS GLN
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ASN ILE GLU GLY GLU TRP GLY ALA PHE ASN ASP ILE MET ARG ARG LYS ASP ILE ALA ASN LEU GLN MET MET LYS ILE VAL GLN GLU 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 GLN ALA LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LYS GLU ALA LEU GLU LEU THR ASP THR GLY LEU LEU SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU GLU LEU Q1327 D1328 E1335 E1341 D1344 Q1345 E1348 W1351 P1356 D1364 K1371 S1372 F1373 L1377 R1378 A1381 R1388 I1396 N1397 M1398 L1399 V1400 I1401 R1411 H1412 W1413 K1414 Q1415 L1416 M1417 K1418 R1419 L1420 H1421 L1429 L1439 Q1440 K1441
K1447 E1456 M1457 A1458 L1459 E1460 E1461 F1462 L1463 K1464 R1467 E1468 V1469 W1470 N1471 Q1481 C1484 R1485 K1496 V1497 K1498 E1499 V1504 M1507 K1514 L1521 E1524 A1532 D1539 V1540 R1543 L1547 E1548 G1549 I1550 F1551 T1552 G1553 K1558 L1561 T1565 Q1566 E1567
I1571 K1581 Q1598 L1601 E1602 R1603 L1604 L1607 I1611 E1620 P1627 R1628 K1649 K1652 I1664 I1665 L1666 I1676 S1677 S1678 R1679 E1680 E1683 I1698 W1701 L1702 V1721 V1724 I1739 L1752 G1771 L1792 Q1800 R1804 D1831
E1871 V1880 Y1889 L1890 T1891 M1892 T1893 F1905 G1906 G1911 K1912 T1913 E1914 R1925 C1932 F1936 M1941 I1944 F1945 V1946 G1947 L1948 V1951 G1952 A1953 W1954 D1958 R1966 M1967 L1968 S1972 Q1979 N1987 P1988 N1989 Y1990 D1991 A1995 P1996 L2002 N2003 K2004 Q2005
V2006 K2007 D2011 T2017 P2020 G2021 TYR ALA GLY ARG S2026 L2035 L2039 A2066 I2069 Q2079 L2080 Q2083 S2084 H2085 K2104 K2112 E2116 E2117 R2118 G2119 E2120 A2121 V2122 D2123 E2126 I2136 L2137 D2153 L2160 F2165 Y2170 C2186 M2189 Y2190
L2191 M2202 V2207 Y2211 L2220 S2228 G2229 K2230 S2231 M2232 A2233 W2234 L2237 L2238 K2239 E2242 A2258 D2269 T2272 R2273 E2274 W2275 T2276 D2277 G2278 T2281 R2285 I2288 D2289 S2290 V2291 R2292 L2295 W2300 D2304 G2305 D2306 V2307 D2320 P2336 P2337 N2338
M2342 F2343 E2344 V2345 A2354 R2358 L2369 I2374 R2383 E2389 G2390 E2391 D2392 E2393 A2394 Q2395 R2396 R2397 ARG LYS GLY LYS GLU ASP GLU GLY E2406 E2407 A2408 M2412 I2415 A2420 M2423 Q2424 C2431 L2432 V2433 T2434 K2435 A2436 L2437 R2451 L2452 R2453 C2454 L2455
P2480 R2488 I2498 L2499 D2505 S2506 R2507 E2516 R2519 R2520 L2526 D2536 Y2537 E2538 G2543 K2551 A2563 V2569 P2570 T2571 L2572 R2576 L2581 V2592 G2619 F2622 S2623 T2644 G2647 F2662 I2666 P2669 R2678 R2694 Q2698


G2710 D2717 R2720 Y2735 I2747 Y2748 G2749 R2757 L2758 I2759 L2762 R2763 T2770 V2774 Y2777 F2784 Y2794 T2800 R2801 R2804 L2810 L2816 E2819 I2822 R2823 D2851 A2854 F2858 I2861 D2862 R2863 A2866 M2867 S2868 V2893 R2896
E2902 D2906 L2911 E2914 V2915 L2916 D2917 H2918 I2925 F2926 R2927 Q2930 L2933 L2934 L2935 T2945 L2946 L2956 I2961 H2964 R2965 K2966 L2980 S2983 K2989 I2990 I2993 M2994 D2995 E2996 S2997 F3004 R3007 T3010 L3011 L3012 E3016 L3020 F3021 E3022
L3042 M3043 L3044 D3045 E3049 V3065 S3071 SER GLU GLY LEU LYS ASP ARG A3079 N3087 L3091 N3092 E3116 P3123 M3126 P3136 P3137 S3138 H3139 R3140 H3155 L3161 G3165 T3168 H3182 E3195 L3201 G3204 Q3214 V3215 E3216 R3220 D3221 LEU
ARG ILE LYS SER GLN GLU LEU GLU VAL LYS ASN ALA ALA ALA ASN ASP LYS LEU LYS LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS 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 ALA VAL ALA GLU VAL ARG SER MET ALA ALA ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU GLU SER ILE CYS LEU LEU LEU GLY GLU SER THR THR ASP TRP LYS GLN GLN ILE ARG SER ILE ILE
MET ARG GLU ASN PHE ILE PRO THR ILE VAL ASN PHE SER ALA GLU GLU ILE SER ASP ALA ILE ARG GLU LYS LYS LYS ASN PRO PRO SER VAL 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 GLN GLN MET ILE ARG ASP LEU GLU ALA SER ILE ALA ARG TYR LYS GLU GLU TYR ALA VAL LEU ILE SER GLU ALA GLN ALA ILE LYS
ALA ASP LEU ALA ALA VAL GLU A3470 R3474 A3477 L3478 L3479 K3480 S3483 R3486 E3487 R3488 W3489 E3490 K3491 T3492 M3500 S3501 T3502 I3503 A3504 G3505 L3508 A3511 I3514 Y3519 R3525 D3546 T3550 S3554 N3576 L3580 K3581 R3582 F3583 N3584 R3585 I3600 M3601
R3611 T3612 S3613 R3620 K3621 L3627 R3628 L3633 V3644 L3649 N3650 R3651 R3655 T3656 R3659 V3660 L3661 G3665 D3666 G3667 D3668 I3669 I3677 R3682 P3690 D3691 R3695 V3696 N3700 V3703 T3704 R3705 L3713 D3730 L3731 L3734 Q3735 G3736 E3746 L3749
L3750 V3756 K3757 G3758 R3759 I3760 L3761 D3762 D3763 D3764 T3765 I3766 I3767 T3768 T3769 L3770 E3771 N3772 L3773 K3774 R3775 E3776 E3779 E3786 E3795 S3798 S3817 L3824 Y3825 S3828 L3829 Q3830 L3833 V3839 L3863 M3875 D3879 F3883 A3888 R3910 S3917 S3920
R3923 I3924 E3933 V3936 R3937 P3942 K3945 E3955 G3958 L3961 P3966 E3977 T3978 D3999 R4000 M4004 M4007 N4012 L4025 D4026 L4027 K4036 P4037 D4057 L4058 N4063 A4074 K4082 A4083 I4084 N4085 V4088 K4097 L4106 K4112
Q4117 P4118 P4135 L4139 I4190 Q4191 E4192 R4193 L4194 R4195 F4207 G4229 W4240 A4248 Q4249 S4250 L4269 T4275 D4289 L4321 P4324 N4325 N4326 R4329 S4341 L4344 K4345 M4346 E4350 D4351 E4352 D4353 ASP LEU ALA TYR ALA GLU THR GLU LYS LYS THR ARG
THR ASP SER THR SER ASP GLY ARG PRO A4375 W4376 H4381 T4382 T4383 N4386 Q4393 T4394 L4395 L4398 K4399 R4400 T4401 K4406 E4414 R4415 E4416 V4417 K4418 M4419 G4420 A4421 K4422 L4423 L4431 C4438 K4443 Q4444 T4445 M4446 R4449 M4453 V4456 K4457 G4458 I4459 L4460 P4461 R4462
S4465 H4466 Y4467 T4468 V4469 P4470 A4471 G4472 S4483 K4487 Q4488 L4489 I4492 A4497 A4501 L4504 S4548 Q4549 G4550 Q4566 T4569 K4574 L4577 S4578 N4579 T4583 A4584 L4585 Q4595 T4596 N4597 T4598 E4599 K4600 A4627 T4628 K4629 F4635 R4638 G4639 V4640 E4646

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67795	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS 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	0.055	Depositor
Minimum map value	-0.020	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: ANP, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.21	0/24934	0.48	8/33786 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3690	PRO	CA-N-CD	-7.32	101.75	112.00
1	A	4418	LYS	CA-CB-CG	6.89	127.89	114.10
1	A	2480	PRO	CA-N-CD	-6.47	102.94	112.00
1	A	3503	ILE	CA-C-N	-6.42	112.46	122.42
1	A	3503	ILE	C-N-CA	-6.42	112.46	122.42

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	24417	0	24462	301	0
2	A	27	0	12	3	0
3	A	31	0	12	3	0
4	A	62	0	26	4	0
All	All	24537	0	24512	304	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 6.

The worst 5 of 304 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:1416:LEU:O	1:A:1420:LEU:HB2	1.81	0.80
1:A:3502:THR:O	1:A:3504:ALA:N	2.22	0.73
1:A:1351:TRP:HB3	1:A:1429:LEU:HB3	1.74	0.70
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	1.75	0.68
1:A:3503:ILE:HG12	1:A:3503:ILE:O	1.93	0.67

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	3020/4646 (65%)	2925 (97%)	92 (3%)	3 (0%)	48 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1996	PRO
1	A	3503	ILE
1	A	1421	HIS

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	2698/4125 (65%)	2684 (100%)	14 (0%)	81 82

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2810	LEU
1	A	3155	HIS
1	A	3703	VAL
1	A	3502	THR
1	A	3503	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4174	ASN
1	A	4231	GLN
1	A	4444	GLN
1	A	2005	GLN
1	A	1979	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ANP	A	4703	-	32,33,33	0.90	4 (12%)	44,52,52	0.90	2 (4%)
3	ATP	A	4702	-	29,33,33	0.34	0	44,52,52	0.45	0
2	ADP	A	4701	-	27,29,29	1.34	4 (14%)	42,45,45	1.97	10 (23%)
4	ANP	A	4704	-	32,33,33	0.89	4 (12%)	44,52,52	0.89	2 (4%)

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	-	-	7/18/38/38	0/3/3/3
3	ATP	A	4702	-	-	2/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
4	ANP	A	4704	-	-	4/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C5-C4	4.38	1.47	1.39
4	A	4703	ANP	PB-O3A	-2.67	1.55	1.59
2	A	4701	ADP	C5-C6	2.60	1.48	1.41
4	A	4704	ANP	PB-O3A	-2.44	1.56	1.59
4	A	4704	ANP	PG-O1G	2.42	1.50	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	ADP	C5-C4-N3	-6.16	118.71	126.75
2	A	4701	ADP	N3-C4-N9	4.77	134.93	127.08
4	A	4704	ANP	PB-O3A-PA	-4.20	117.84	132.62
2	A	4701	ADP	C2-N3-C4	4.00	121.20	111.75
4	A	4703	ANP	PB-O3A-PA	-3.99	118.56	132.62

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PA-O3A-PB-O1B
4	A	4703	ANP	PA-O3A-PB-O2B
4	A	4703	ANP	C5'-O5'-PA-O3A
4	A	4704	ANP	PG-N3B-PB-O1B
4	A	4704	ANP	PG-N3B-PB-O3A

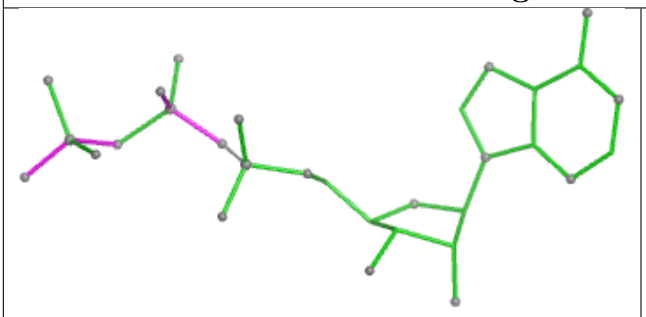
There are no ring outliers.

4 monomers are involved in 10 short contacts:

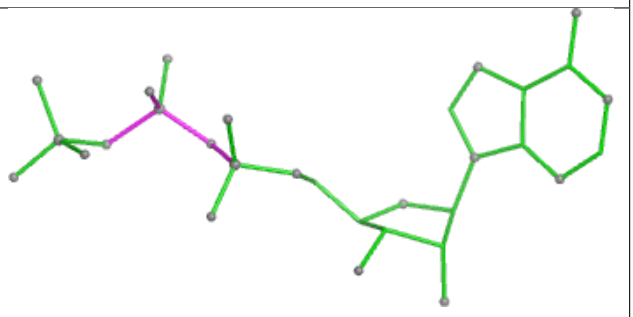
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	2	0
3	A	4702	ATP	3	0
2	A	4701	ADP	3	0
4	A	4704	ANP	2	0

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.

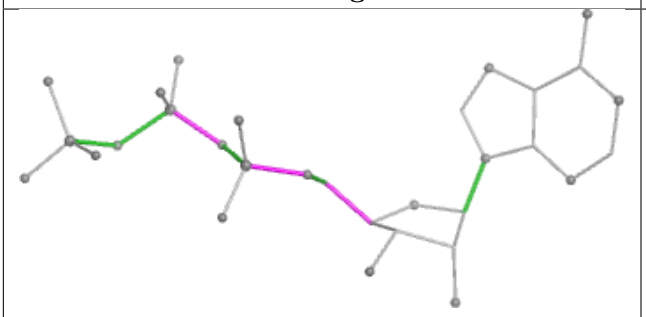
Ligand ANP A 4703



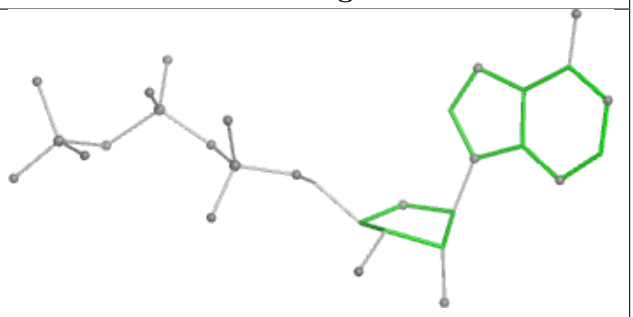
Bond lengths



Bond angles

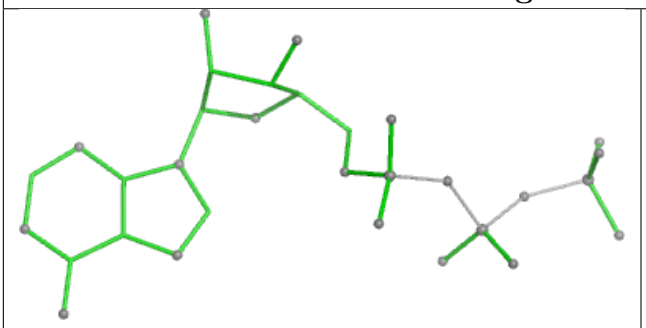


Torsions

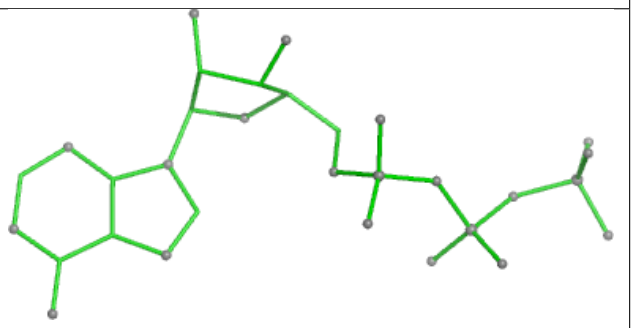


Rings

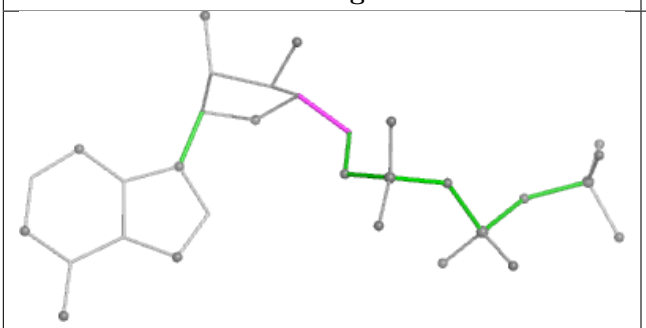
Ligand ATP A 4702



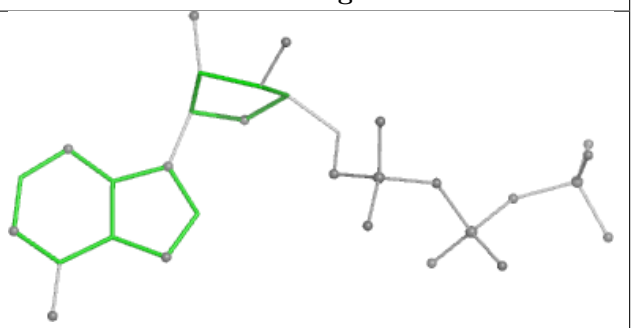
Bond lengths



Bond angles

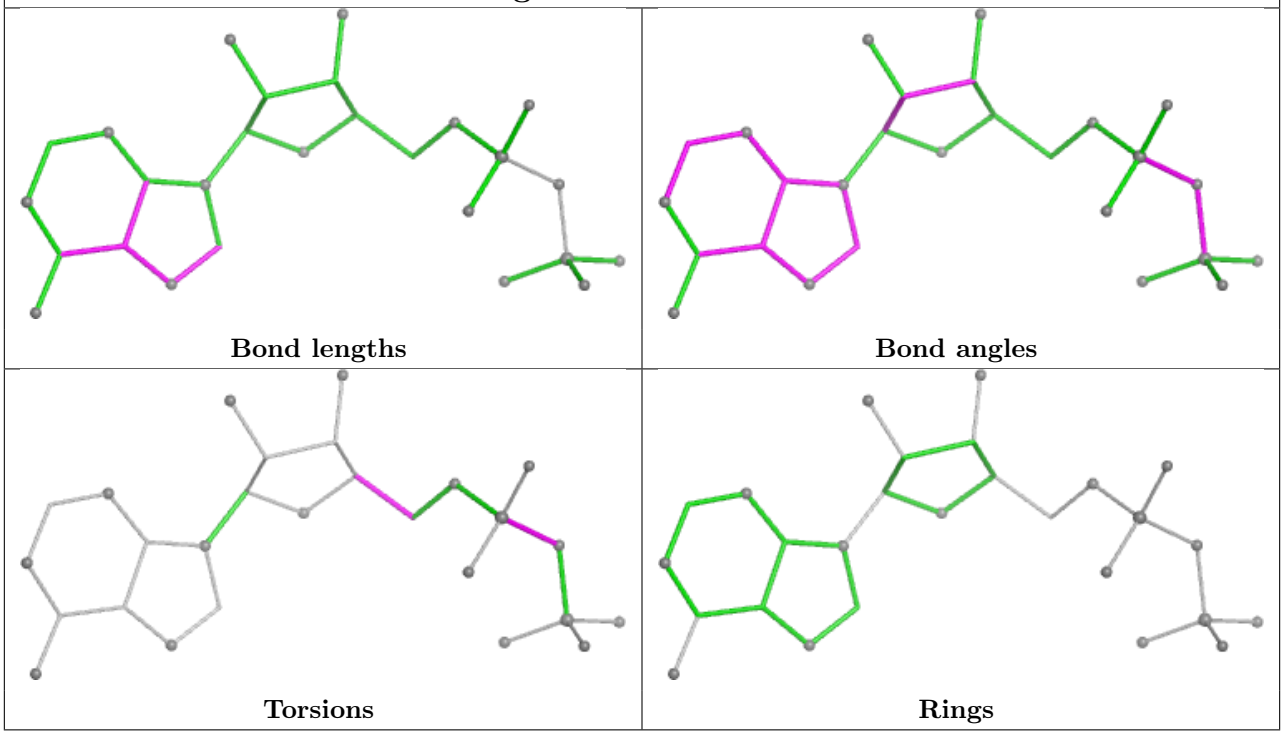


Torsions

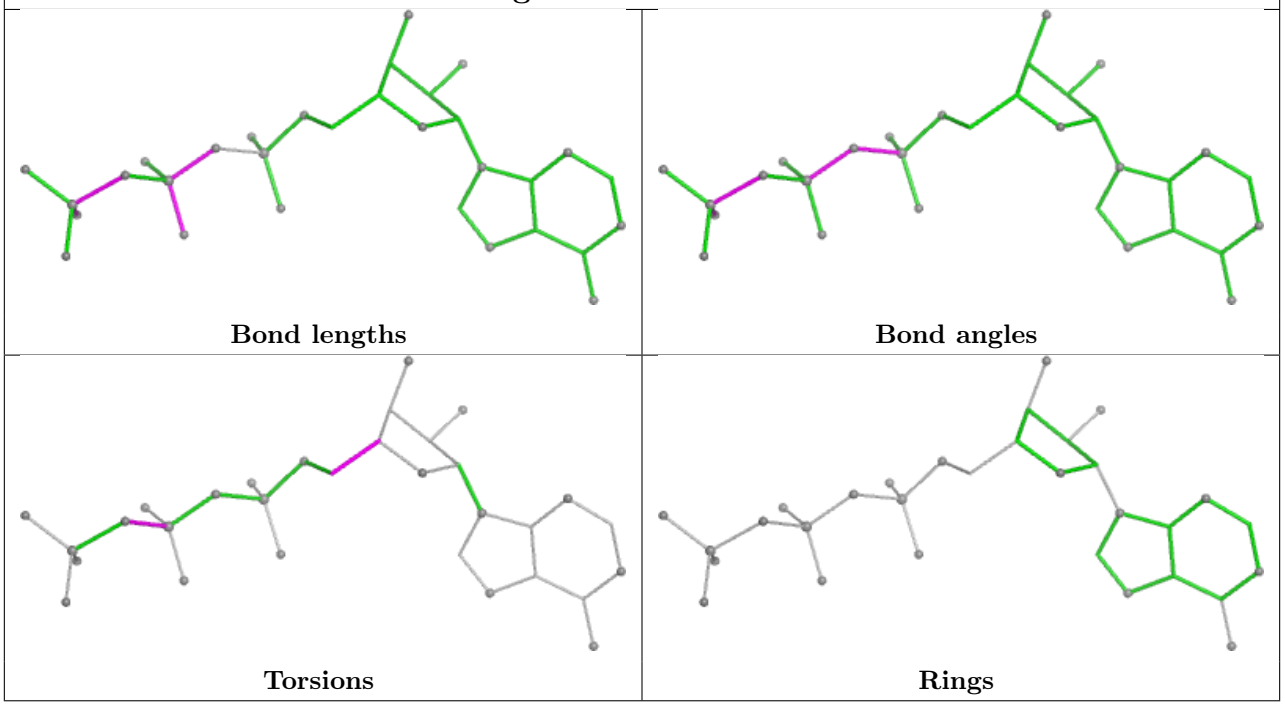


Rings

Ligand ADP A 4701



Ligand ANP A 4704



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.

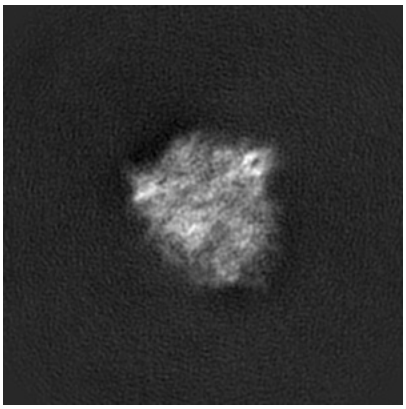
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17825. These allow visual inspection of the internal detail of the map and identification of artifacts.

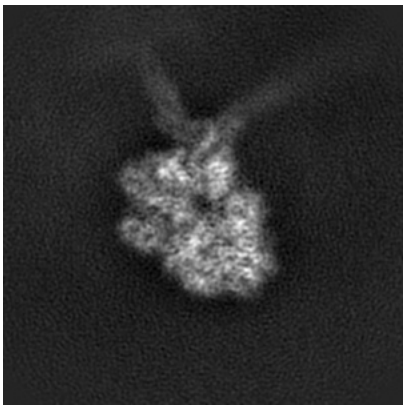
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

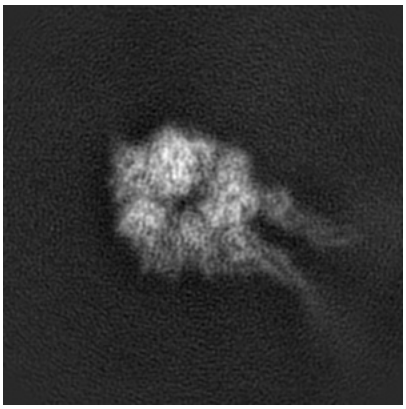
6.1.1 Primary map



X

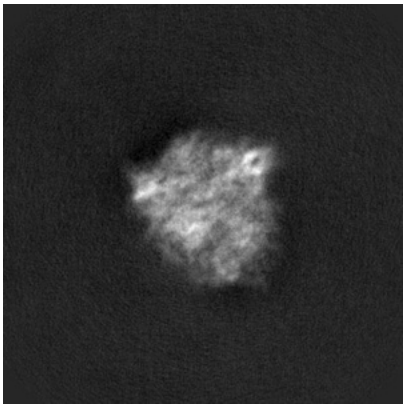


Y

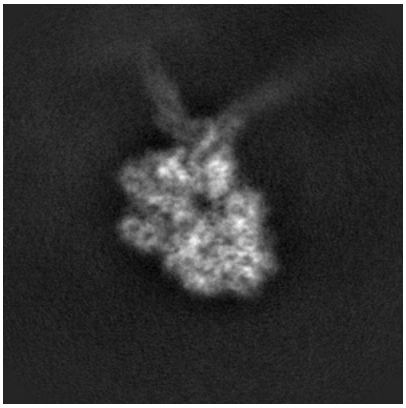


Z

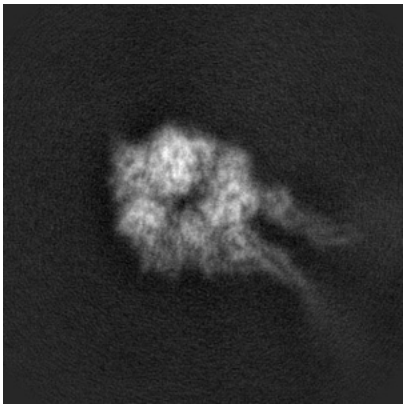
6.1.2 Raw map



X



Y

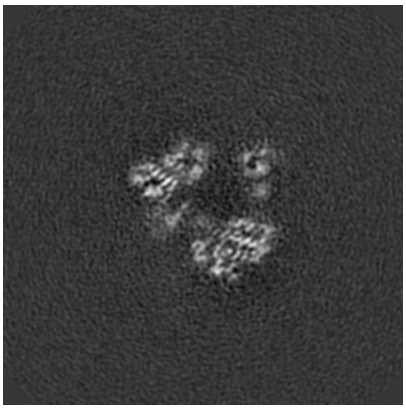


Z

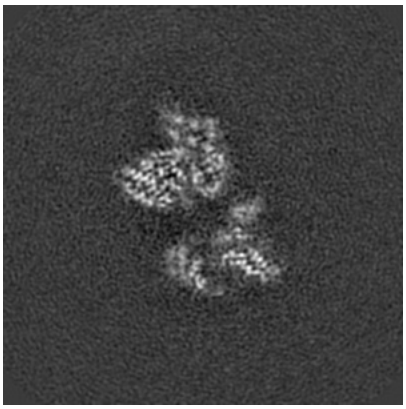
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

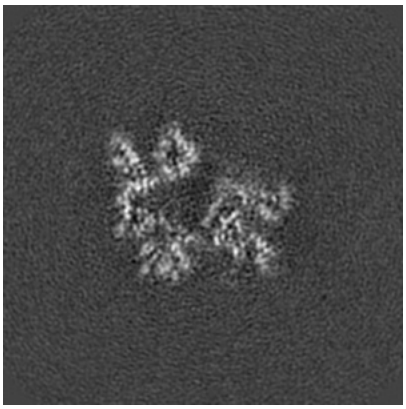
6.2.1 Primary map



X Index: 140

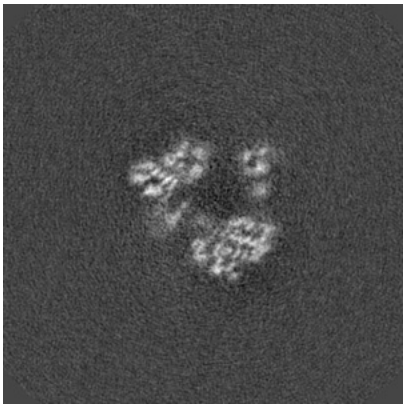


Y Index: 140

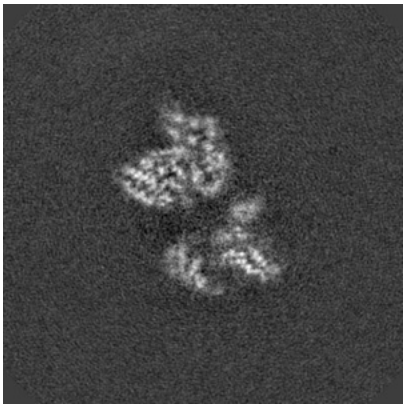


Z Index: 140

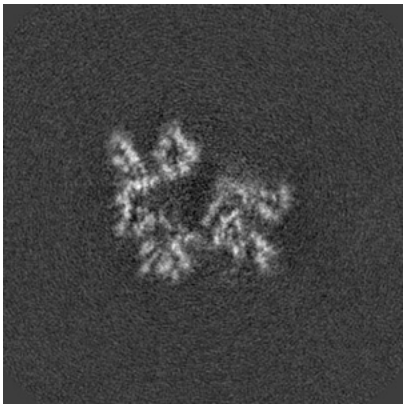
6.2.2 Raw map



X Index: 140



Y Index: 140

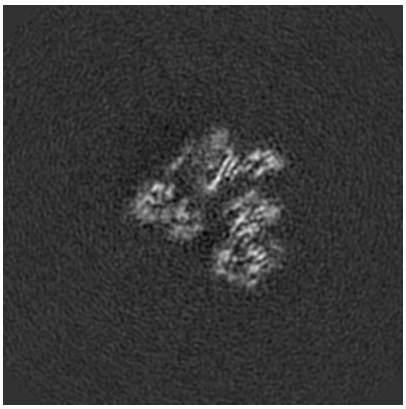


Z Index: 140

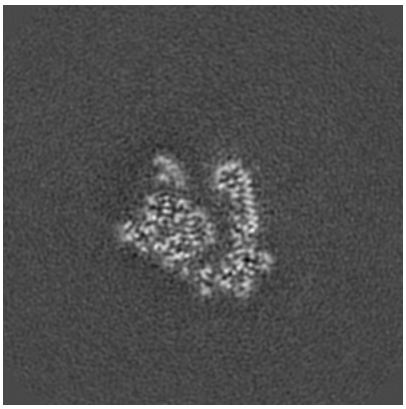
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

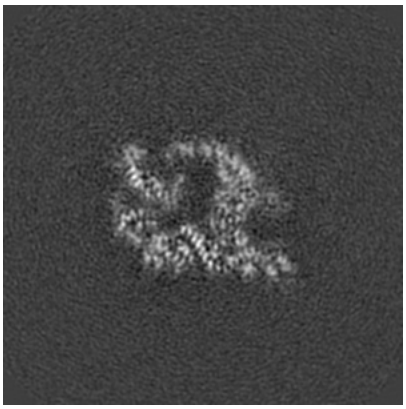
6.3.1 Primary map



X Index: 114

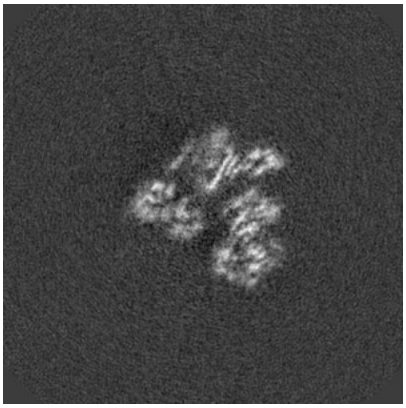


Y Index: 170

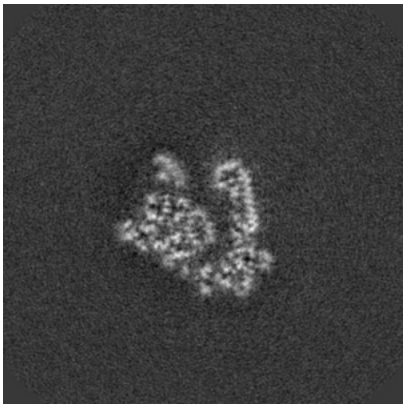


Z Index: 150

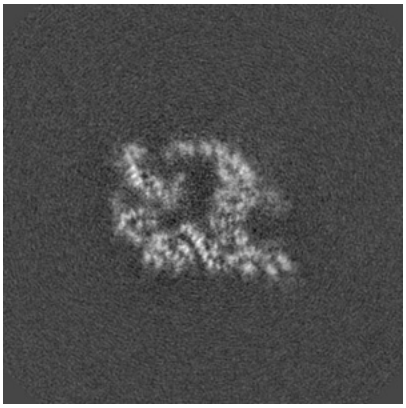
6.3.2 Raw map



X Index: 114



Y Index: 170

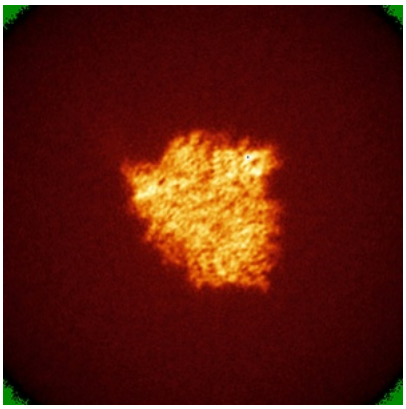


Z Index: 150

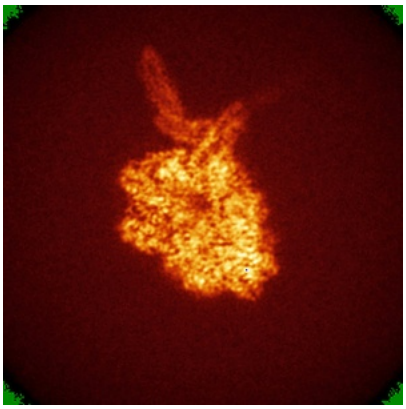
The images above show the largest variance slices of the map in three orthogonal directions.

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

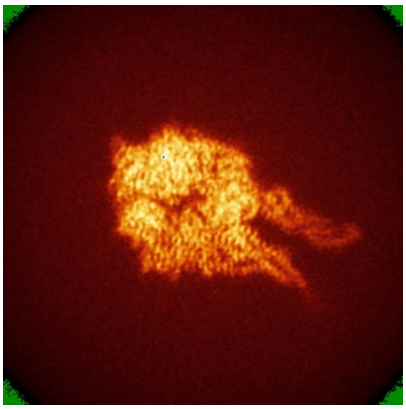
6.4.1 Primary map



X

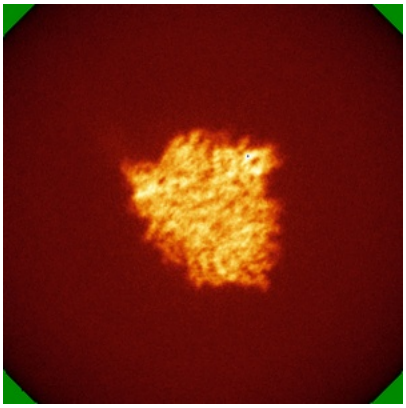


Y

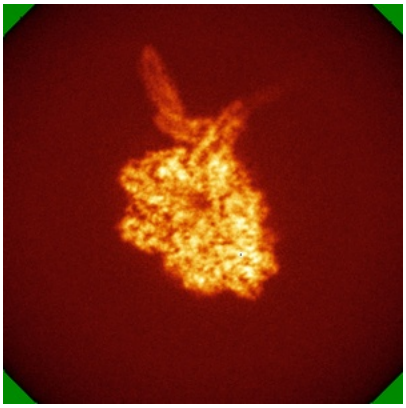


Z

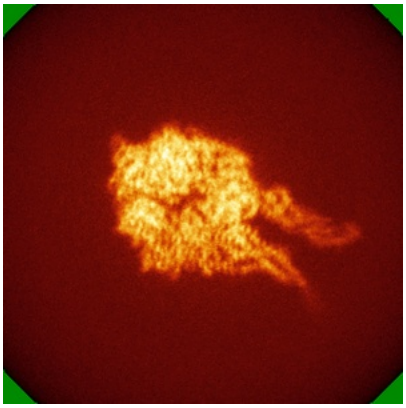
6.4.2 Raw map



X



Y

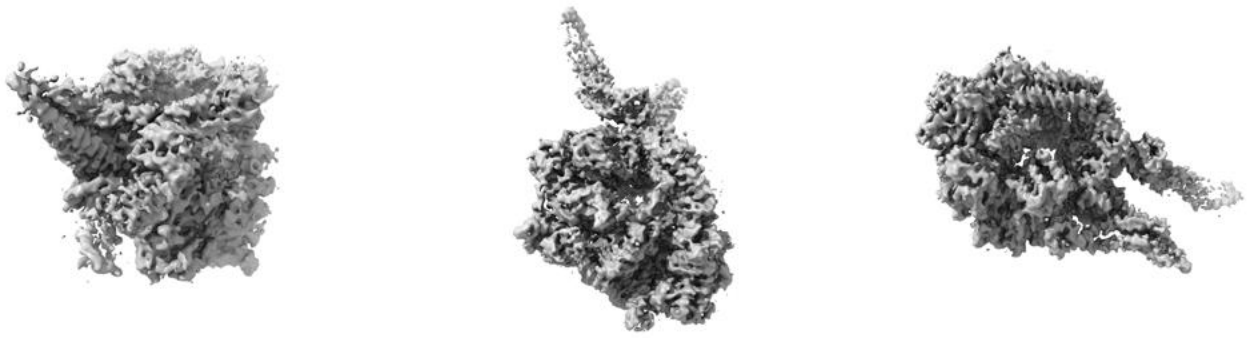


Z

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)

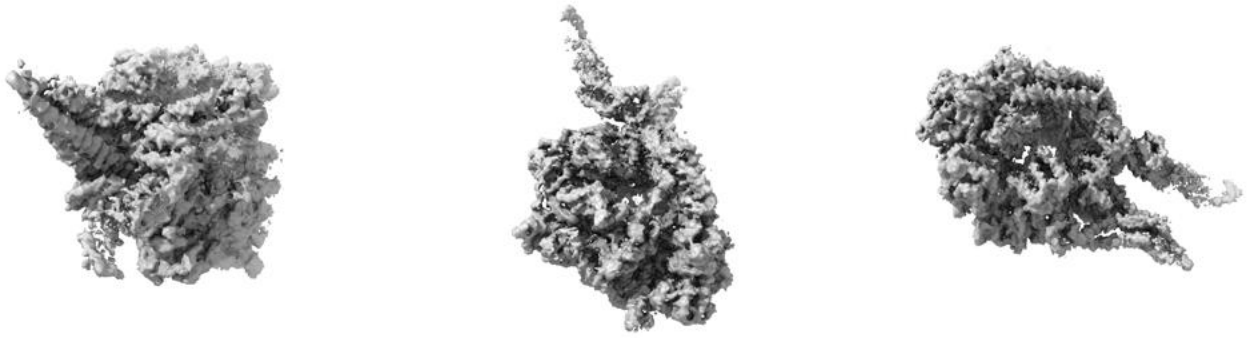
6.5.1 Primary map



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.

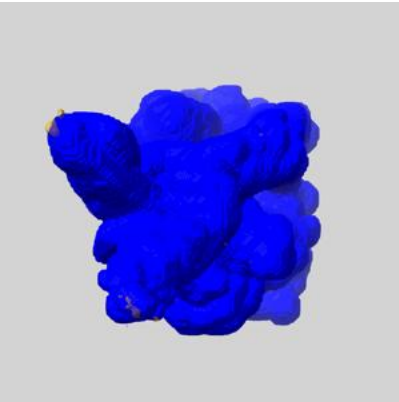
6.6 Mask visualisation (i)

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

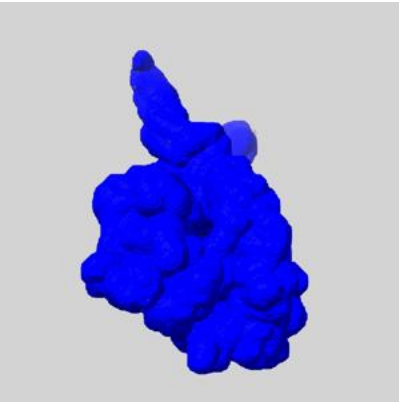
A mask typically either:

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

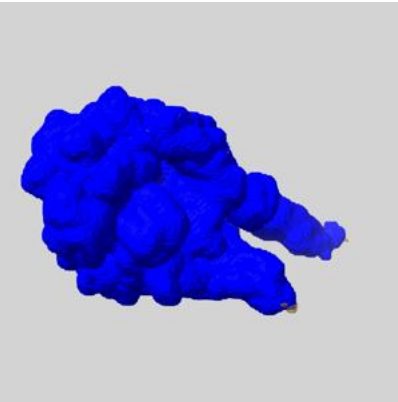
6.6.1 emd_17825_msk_1.map (i)



X



Y

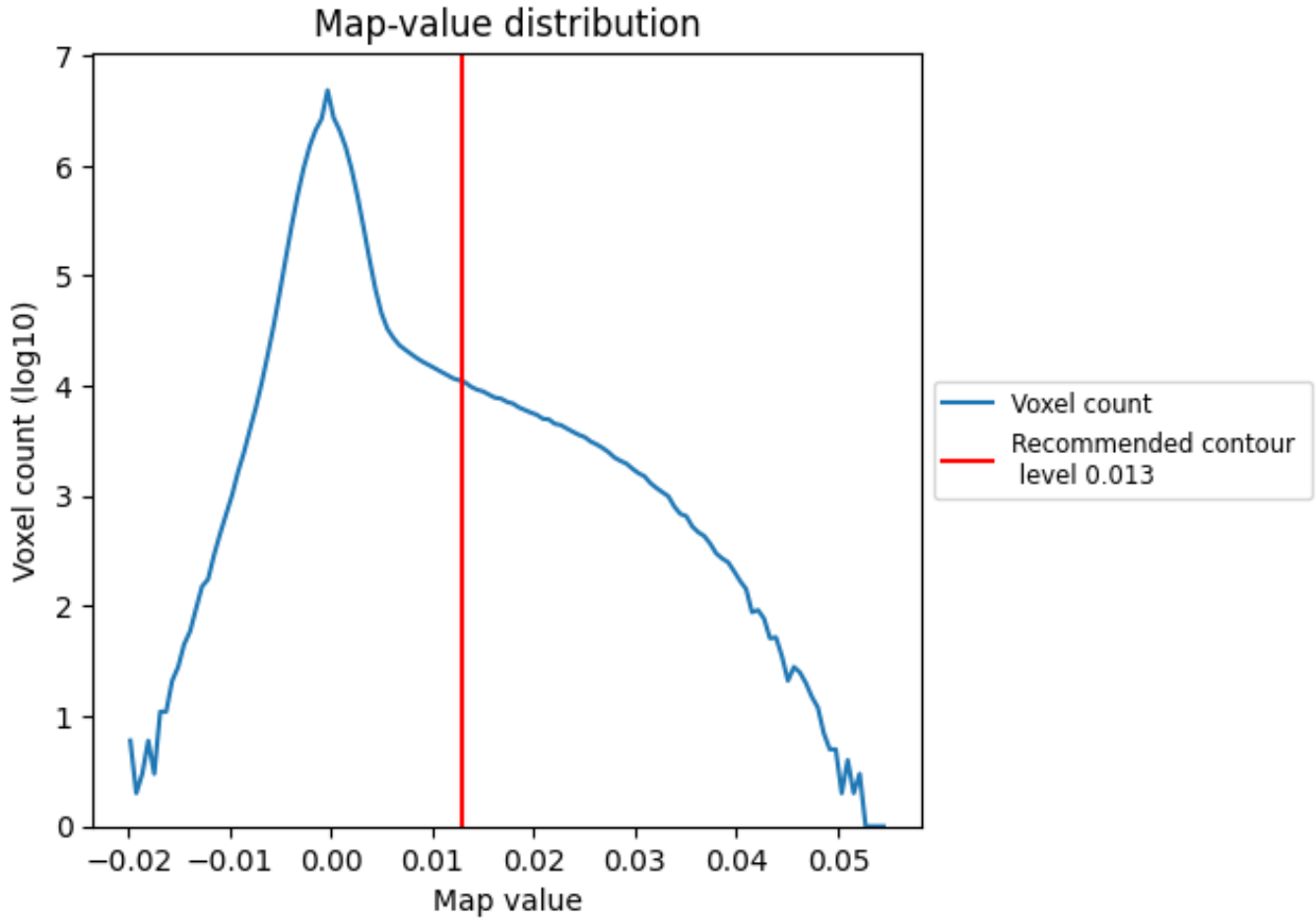


Z

7 Map analysis

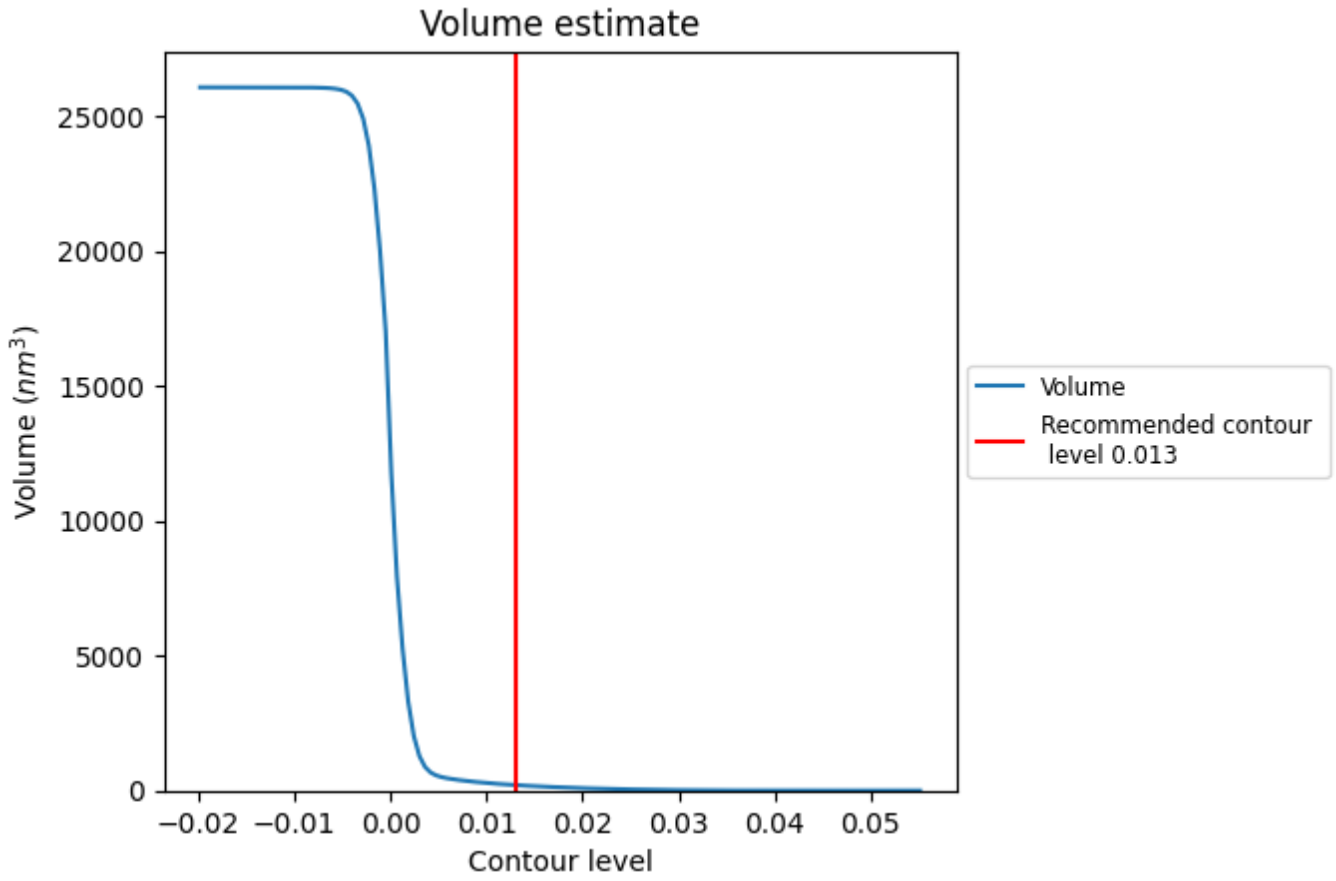
This section contains the results of statistical analysis of the map.

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.

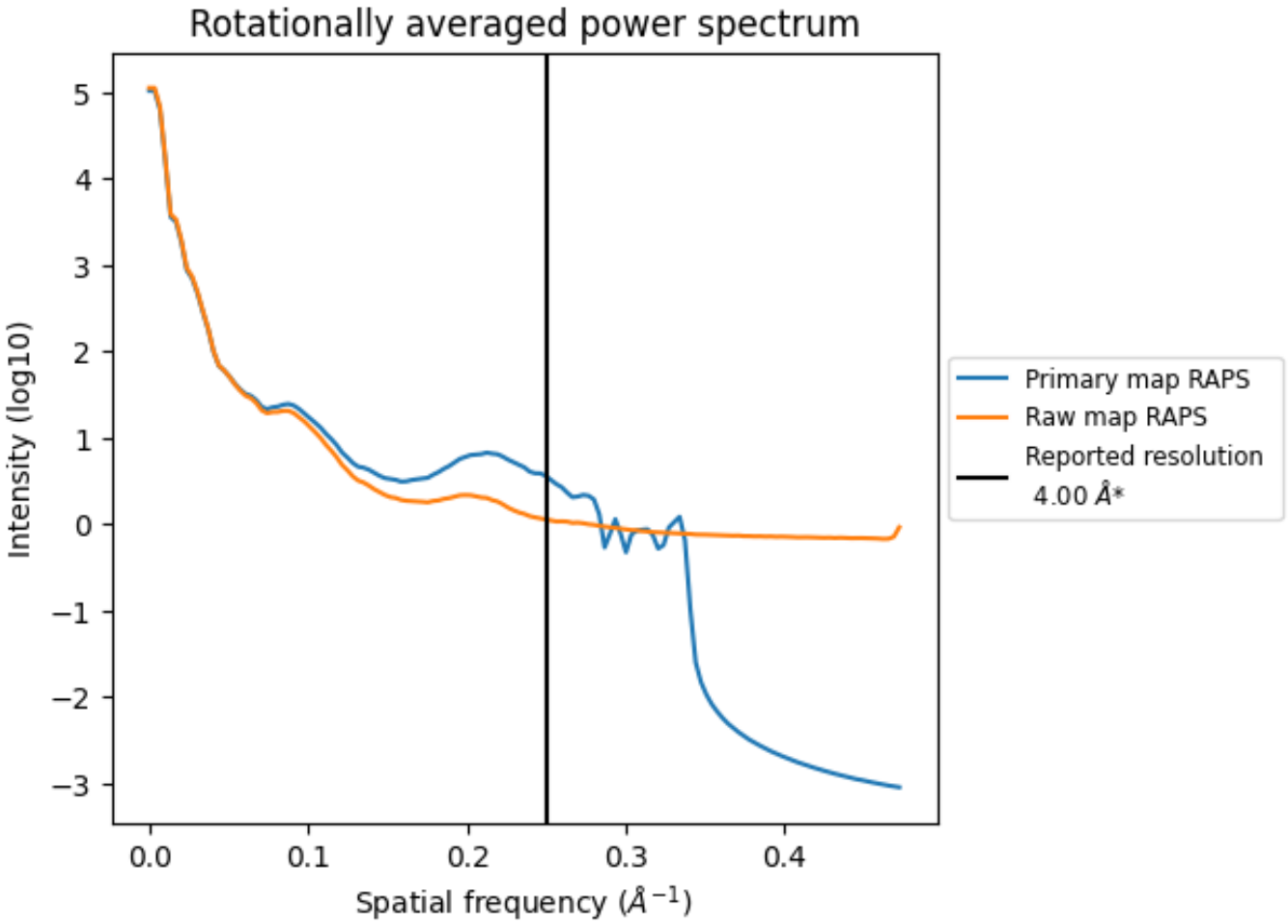
7.2 Volume estimate (i)



The volume at the recommended contour level is 203 nm^3; this corresponds to an approximate mass of 184 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)

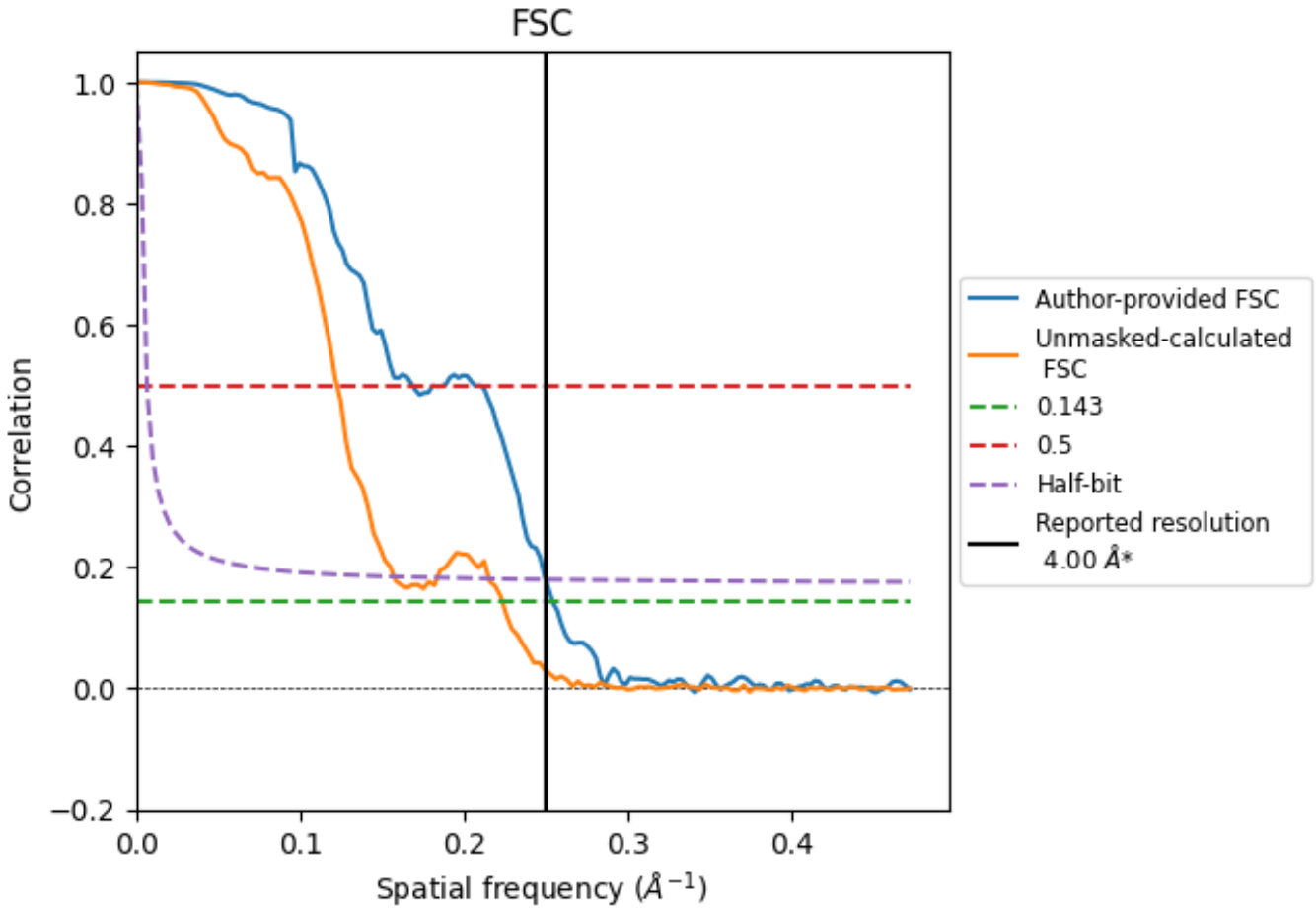


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

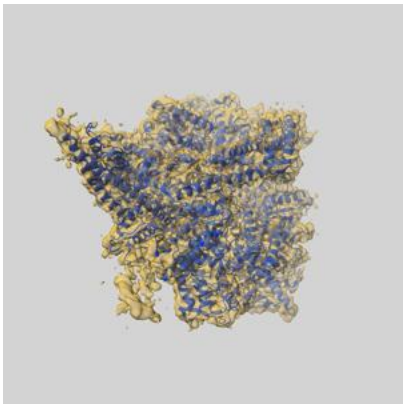
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.93	5.93	4.00
Unmasked-calculated*	4.47	8.16	6.35

*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 4.47 differs from the reported value 4.0 by more than 10 %

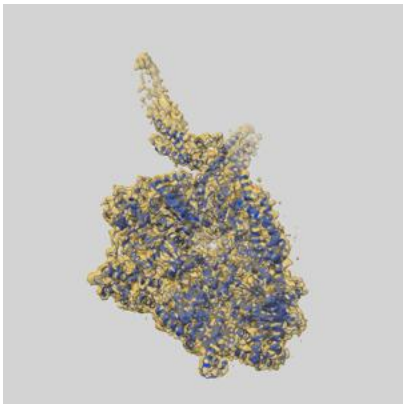
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17825 and PDB model 8PQV. Per-residue inclusion information can be found in section 3 on page 5.

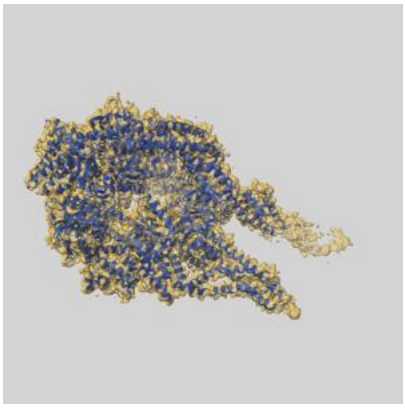
9.1 Map-model overlay



X



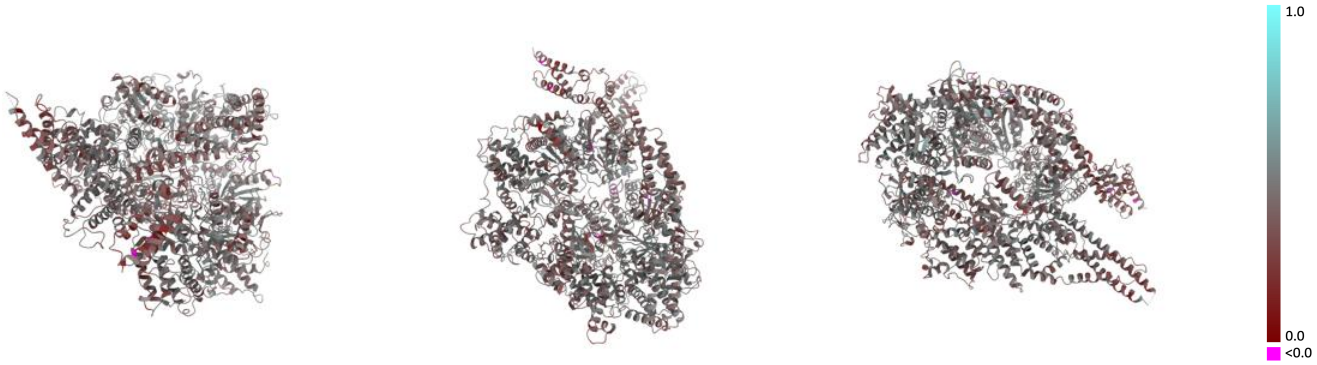
Y



Z

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

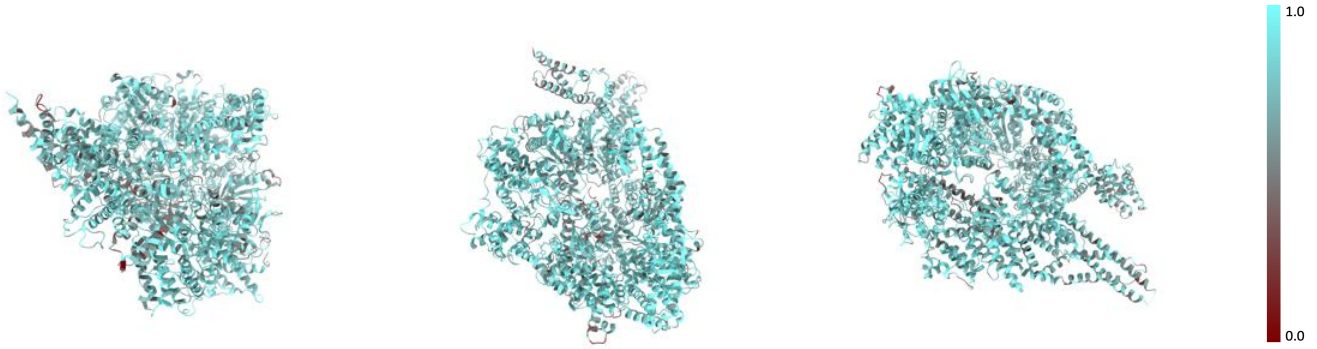
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

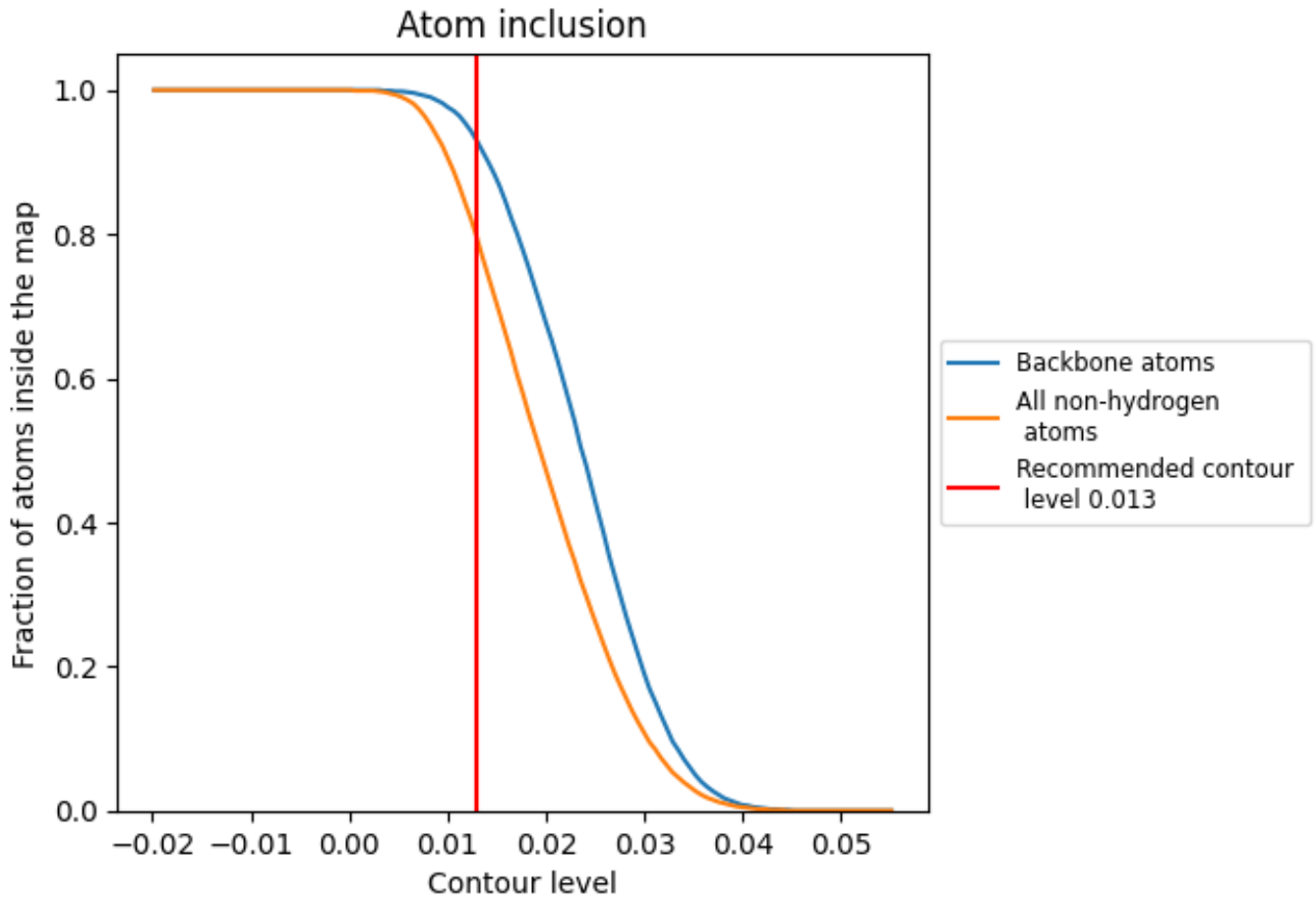
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 79% 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	0.7940	0.4170
A	0.7940	0.4170