Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 10:44 AM EDT

PDB ID	:	9BMM / pdb_00009bmm
EMDB ID	:	EMD-44703
Title	:	State-4 of the motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.10 Å(reported)

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

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

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

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

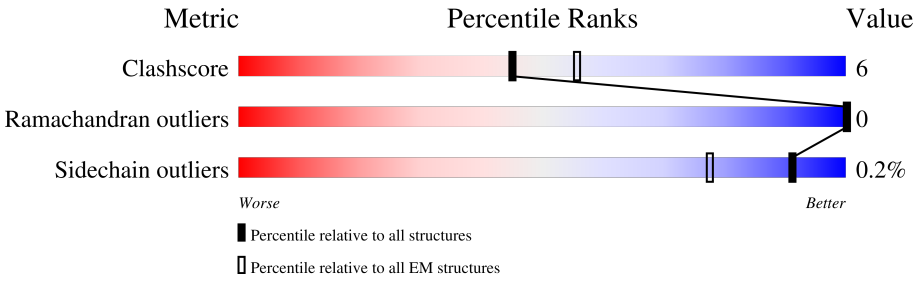
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	52% 10% 38%

2 Entry composition

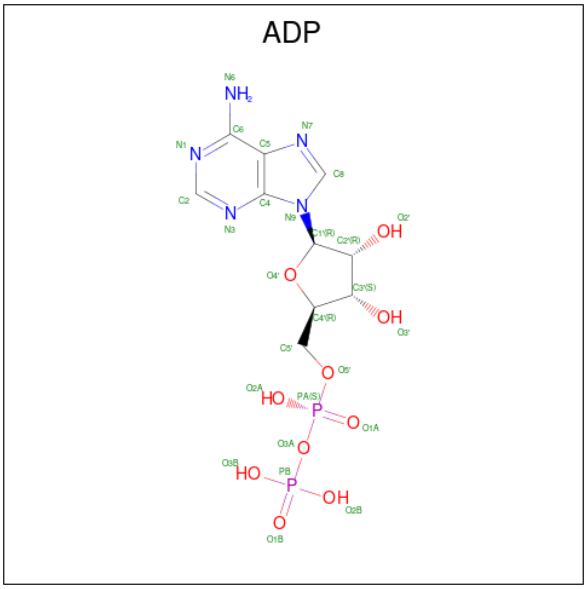
There are 4 unique types of molecules in this entry. The entry contains 23038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

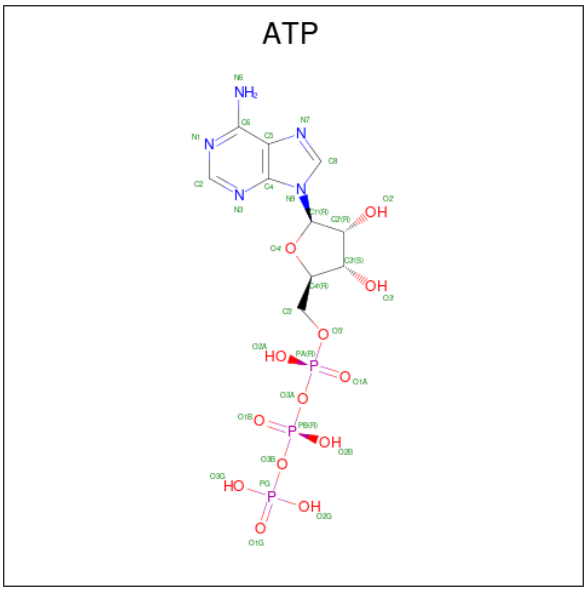
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2859	22925	14595	3960	4257	113	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
			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 MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

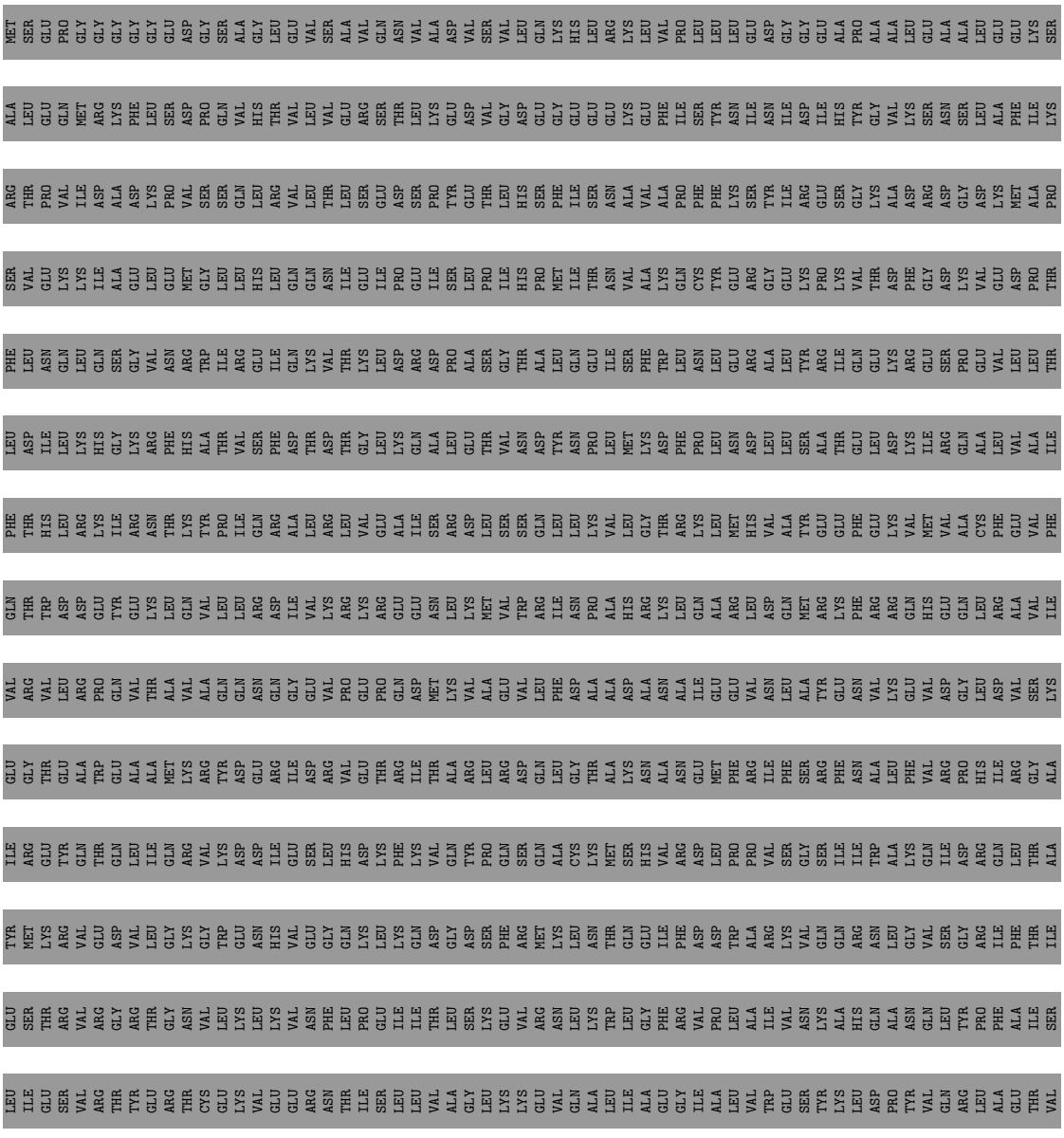
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

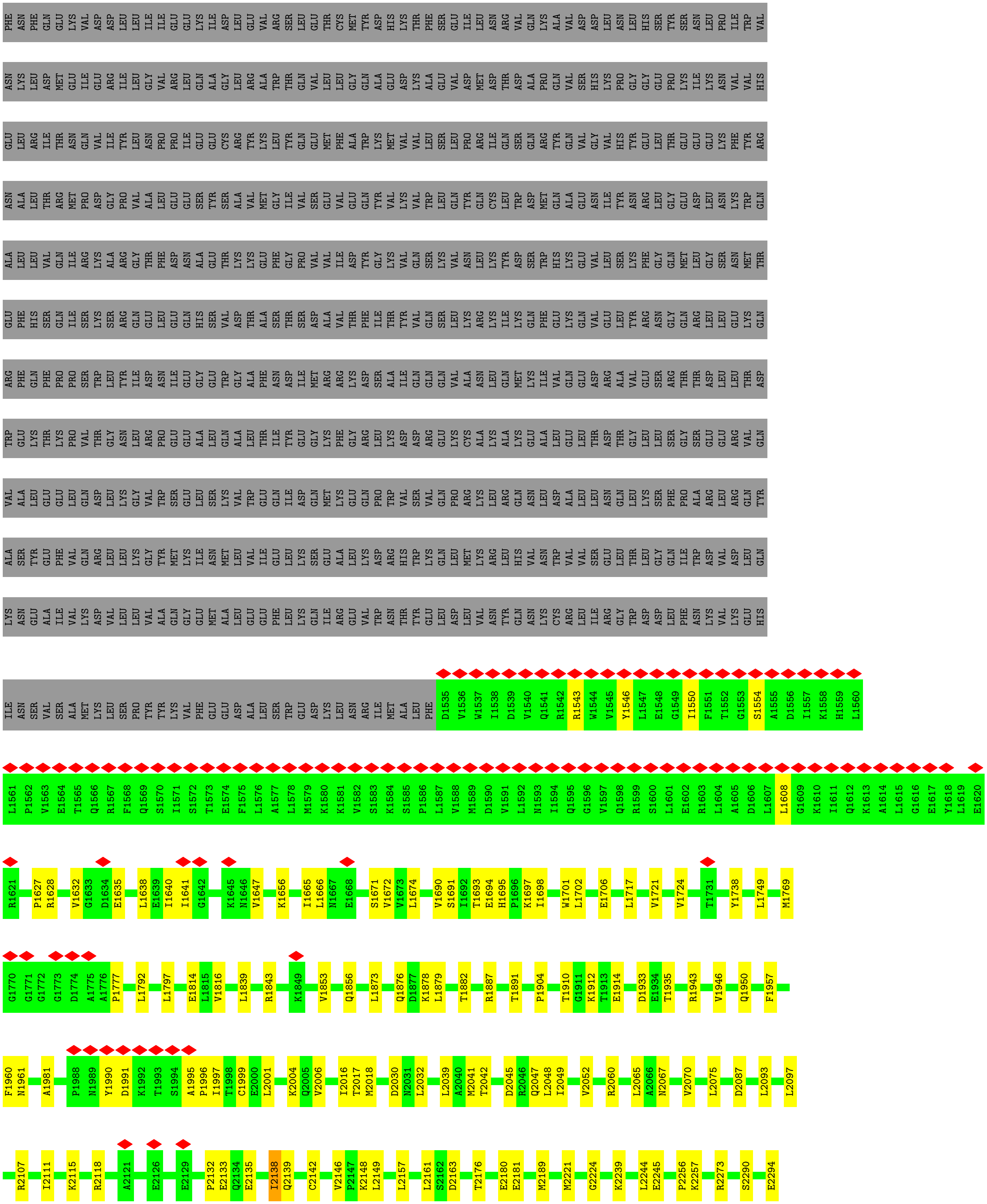
3 Residue-property plots (i)

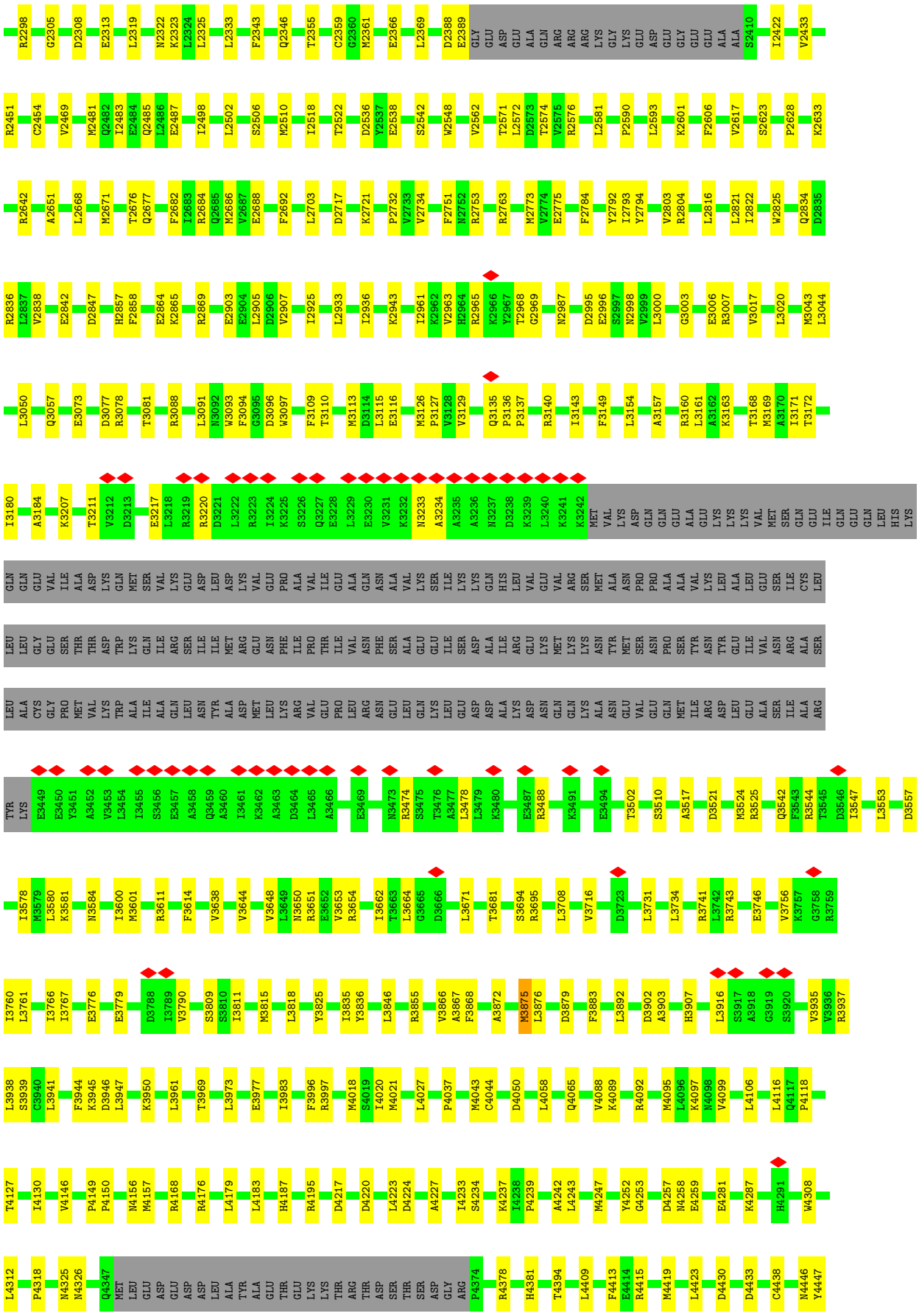
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 TRP VAL
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 SER LEU PRO ARG ILE GLN SER GLN ARG TYR GLN VAL GLY VAL HIS TYR GLU LEU THR GLU 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 GLU GLN TYR VAL LYS VAL TRP 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 LEU 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 GLN SER LEU LYS ARG LYS ILE LYS GLN PHE GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN ARG LEU LEU GLU 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 SER ALA ILE GLN GLN GLN VAL ALA ASN LEU GLN MET LYS ILE VAL GLN 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 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 GLY SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU GLU LEU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU SER LYS VAL TRP GLU 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 SER PHE PRO ALA ARG LEU ARG GLN TYR
ALA SER TYR GLU PHE VAL GLN ARG LEU LEU 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 ALA ILE VAL LYS ASP VAL LEU LEU VAL ALA GLN GLY GLU MET ALA LEU GLU GLU PHE LEU LYS GLN ILE ARG GLU VAL TRP ASN THR TYR GLU LEU ASP LEU VAL ASN TYR GLN ASN LYS CYS ARG LEU ILE ARG GLY TRP ASP ASP LEU PHE ASN LYS VAL LYS GLU HIS
ILE ASN SER VAL SER ALA MET LYS LEU SER PRO TYR TYR LYS VAL PHE GLU GLU ASP ALA LEU SER TRP GLU ASP LYS LEU ASN ARG ILE MET ALA LEU PHE D1535 V1536 W1537 I1538 D1539 V1540 Q1541 R1542 R1543 W1544 V1545 Y1546 L1547 E1548 G1549 I1550 F1551 T1552 G1553 S1554 A1555 D1556 I1557 K1558 H1559 L1560
L1561 P1562 V1563 E1564 T1565 Q1566 R1567 F1568 Q1569 S1570 I1571 S1572 T1573 E1574 F1575 L1576 A1577 L1578 M1579 K1580 K1581 V1582 S1583 K1584 S1585 P1586 L1587 V1588 M1589 D1590 V1591 L1592 N1593 I1594 Q1595 G1596 V1597 Q1598 R1599 S1600 L1601 E1602 R1603 L1604 A1605 D1606 L1607 L1608 G1609 K1610 I1611 Q1612 K1613 A1614 L1615 G1616 E1617 Y1618 L1619 E1620
R1621 P1627 R1628 V1632 G1633 D1634 E1635 L1638 E1639 I1640 I1641 G1642 K1645 N1646 V1647 K1656 I1665 L1666 N1667 E1668 S1671 V1672 V1673 L1674 V1690 S1691 I1692 T1693 E1694 H1695 P1696 K1697 I1698 W1701 L1702 E1706 L1717 V1721 V1724 T1731 Y1738 L1749 M1769
G1770 G1771 G1772 G1773 D1774 A1775 A1776 P1777 L1792 L1797 E1814 L1815 V1816 L1839 R1843 K1849 V1853 Q1856 L1873 Q1876 D1877 K1878 L1879 T1882 R1887 T1891 P1904 T1910 G1911 K1912 T1913 E1914 D1933 E1934 T1935 R1943 V1946 Q1950 F1957
F1960 N1961 A1981 P1988 N1989 Y1990 D1991 K1992 T1993 S1994 A1995 P1996 I1997 T1998 C1999 E2000 L2001 K2004 Q2005 V2006 I2016 T2017 M2018 D2030 N2031 L2032 L2039 A2040 M2041 T2042 D2045 R2046 Q2047 L2048 I2049 V2052 R2060 L2065 A2066 N2067 V2070 L2075 D2087 L2093 L2097
R2107 I2111 K2115 R2118 A2121 E2126 E2129 P2132 E2133 Q2134 E2135 I2138 Q2139 C2142 V2146 P2147 K2148 L2149 L2157 L2161 S2162 D2163 T2176 E2180 E2181 M2189 M2221 G2224 K2239 L2244 E2245 P2256 K2257 R2273 S2290 E2294


R2298 G2305 D2308 E2313 L2319 N2322 K2323 L2324 L2325 L2333 F2343 Q2346 T2355 C2359 G2360 M2361 E2366 L2369 D2388 E2389 GLY GLU ASP GLU ALA GLN ARG ARG ARG LYS GLY LYS GLU ASP GLU GLY GLU GLU GLU ALA S2410 I2422 V2433
R2451 C2454 V2469 M2481 Q2482 I2483 E2484 Q2485 L2486 E2487 I2498 L2502 S2506 M2510 I2518 T2522 D2536 Y2537 E2538 S2542 W2548 V2562 T2571 L2572 D2573 T2574 V2575 R2576 L2581 P2590 L2593 K2601 F2606 V2617 S2623 P2628 K2633
R2642 A2651 L2668 M2671 T2676 Q2677 F2682 I2683 R2684 Q2685 M2686 V2687 E2688 F2692 L2703 D2717 K2721 P2732 V2733 V2734 F2751 N2752 R2753 R2763 M2773 V2774 E2775 F2784 Y2792 I2793 Y2794 V2803 R2804 L2816 L2821 I2822 W2825 Q2834 D2835
R2836 L2837 V2838 E2842 D2847 H2857 F2858 E2864 K2865 R2869 E2903 E2904 L2905 D2906 V2907 I2925 L2933 I2936 K2943 I2961 K2962 V2963 H2964 R2965 K2966 Y2967 T2968 G2969 N2987 D2995 E2996 S2997 N2998 V2999 L3000 G3003 E3006 R3007 V3017 L3020 M3043 L3044
L3050 Q3057 E3073 D3077 R3078 T3081 R3088 L3091 N3092 W3093 F3094 G3095 D3096 W3097 F3109 T3110 M3113 D3114 L3115 E3116 M3126 P3127 V3128 V3129 Q3135 P3136 P3137 R3140 I3143 F3149 L3154 A3157 R3160 L3161 A3162 K3163 T3168 M3169 A3170 I3171 T3172
I3180 A3184 K3207 T3211 V3212 D3213 E3217 L3218 R3219 R3220 D3221 L3222 R3223 I3224 K3225 S3226 Q3227 E3228 L3229 E3230 V3231 K3232 N3233 A3234 A3235 A3236 N3237 D3238 K3239 L3240 K3241 K3242 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 VAL ASN PHE SER ALA GLU GLU ILE SER ASP ALA ILE ARG GLU LYS MET LYS LYS ASN TYR MET SER ASN PRO SER TYR ASN TYR GLU ILE VAL ASN ARG ALA SER
LEU ALA CYS GLY PRO MET VAL LYS TRP ALA ILE ALA 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 E3449 E3450 Y3451 A3452 V3453 L3454 I3455 S3456 E3457 A3458 Q3459 A3460 I3461 K3462 A3463 D3464 L3465 A3466 E3469 N3473 R3474 S3475 T3476 A3477 L3478 L3479 K3480 E3487 R3488 K3491 E3494 T3502 S3510 A3517 D3521 M3524 R3525 Q3542 F3543 R3544 T3545 D3546 I3547 L3553 D3557
I3578 M3579 L3580 K3581 N3584 I3600 M3601 R3611 F3614 V3638 V3644 V3648 L3649 N3650 R3651 E3652 V3653 R3654 I3662 T3663 L3664 G3665 D3666 L3671 T3681 S3694 R3695 L3708 V3716 D3723 L3731 L3734 R3741 L3742 R3743 E3746 V3756 K3757 G3758 R3759
I3760 L3761 I3766 I3767 E3776 E3779 D3788 I3789 V3790 S3809 S3810 I3811 M3815 L3818 Y3825 I3835 Y3836 L3846 R3855 V3866 A3867 F3868 A3872 M3875 L3876 D3879 F3883 L3892 D3902 A3903 H3907 L3916 S3917 A3918 G3919 S3920 V3935 V3936 R3937
L3938 S3939 C3940 L3941 F3944 K3945 D3946 L3947 K3950 L3961 T3969 L3973 E3977 I3983 F3996 R3997 M4018 S4019 I4020 M4021 L4027 P4037 M4043 C4044 D4050 L4058 Q4065 V4088 K4089 R4092 M4095 L4096 K4097 N4098 V4099 L4106 L4116 Q4117 P4118
T4127 I4130 V4146 P4149 P4150 N4156 M4157 R4168 R4176 L4179 L4183 H4187 R4195 D4217 D4220 L4223 D4224 A4227 I4233 S4234 K4237 T4238 P4239 A4242 L4243 M4247 Y4252 G4253 D4257 N4258 E4259 E4281 K4287 H4291 W4308
L4312 P4318 N4325 N4326 Q4347 MET LEU GLU ASP GLU ASP ASP LEU ALA TYR ALA GLU THR GLU LYS LYS THR ARG THR ASP SER THR SER ASP GLY ARG P4374 R4378 H4381 T4394 L4409 F4413 E4414 R4415 M4419 L4423 D4430 D4433 C4438 N4446 Y4447


L4448
L4460
P4461
S4465
H4466
V4475
L4489
Q4490
L4504
K4505
F4515
T4522
S4535
L4536
E4537
L4541
E4542
V4543
Q4549
D4554
F4558
N4579
T4588
Q4589
L4590
N4597
T4598
E4599
K4629
T4645
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92310	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.145	Depositor
Minimum map value	-1.237	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	0.17	0/23409	0.30	0/31728

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22925	0	22998	280	0
2	A	81	0	36	3	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	23038	0	23046	280	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.

All (280) 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:2221:MET:HG2	1:A:2343:PHE:HB2	1.63	0.81
1:A:2115:LYS:HD2	1:A:2118:ARG:HH21	1.46	0.79
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.62	0.79
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.66	0.76
1:A:2834:GLN:NE2	1:A:2847:ASP:OD2	2.21	0.74
1:A:1882:THR:HG21	1:A:2049:ILE:HG13	1.76	0.66
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.29	0.65
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.27	0.65
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.79	0.64
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.62	0.64
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.29	0.64
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.80	0.63
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.80	0.63
1:A:1814:GLU:HB2	1:A:1878:LYS:NZ	2.13	0.63
1:A:1797:LEU:HD21	1:A:2060:ARG:HD3	1.81	0.62
1:A:3907:HIS:CG	1:A:3941:LEU:HD11	2.34	0.62
1:A:2290:SER:HB2	1:A:2294:GLU:H	1.65	0.62
1:A:2684:ARG:NH1	1:A:2688:GLU:OE1	2.33	0.62
1:A:2469:VAL:HG13	1:A:2481:MET:HE2	1.81	0.61
1:A:2115:LYS:HD2	1:A:2118:ARG:NH2	2.14	0.61
1:A:3154:LEU:HB3	1:A:3171:ILE:HG13	1.82	0.61
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.83	0.61
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.33	0.61
1:A:3488:ARG:NH1	1:A:3746:GLU:OE1	2.34	0.60
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.82	0.60
1:A:3116:GLU:OE1	1:A:3140:ARG:NH2	2.29	0.60
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.36	0.59
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.85	0.58
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.32	0.58
1:A:3474:ARG:HE	1:A:3767:ILE:HG21	1.68	0.58
1:A:1981:ALA:O	1:A:1997:ILE:HG21	2.02	0.58
1:A:2773:MET:HE1	1:A:2803:VAL:HG22	1.84	0.58
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.85	0.57
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.87	0.57
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.86	0.57
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.86	0.57
1:A:1672:VAL:HA	1:A:1691:SER:HA	1.85	0.57
1:A:2996:GLU:HG3	1:A:3078:ARG:HH12	1.70	0.57
1:A:2717:ASP:O	1:A:4446:ASN:ND2	2.37	0.57
1:A:3044:LEU:HD12	1:A:3050:LEU:HD23	1.86	0.57
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.38	0.56
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	1.88	0.56
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.88	0.56
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.39	0.56
1:A:3644:VAL:HG22	1:A:3664:LEU:HD22	1.87	0.56
1:A:2686:MET:HE3	1:A:2703:LEU:HD11	1.88	0.56
1:A:4433:ASP:HB3	1:A:4448:LEU:HD11	1.87	0.55
1:A:2968:THR:OG1	1:A:2969:GLY:N	2.38	0.55
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.07	0.55
1:A:2686:MET:HG2	1:A:2692:PHE:HB3	1.88	0.55
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	1.88	0.55
1:A:2995:ASP:OD2	1:A:2996:GLU:N	2.40	0.54
1:A:1550:ILE:O	1:A:1554:SER:OG	2.23	0.54
1:A:2163:ASP:HB3	1:A:4536:LEU:HD23	1.90	0.54
1:A:2030:ASP:HB3	1:A:4050:ASP:HB2	1.88	0.54
1:A:2111:ILE:HG23	1:A:2115:LYS:HE3	1.89	0.54
1:A:3113:MET:HE3	1:A:3115:LEU:HD21	1.89	0.54
1:A:1698:ILE:O	1:A:1702:LEU:HB2	2.08	0.54
1:A:3544:ARG:HD3	1:A:3547:ILE:HB	1.90	0.54
1:A:4065:GLN:HB3	1:A:4092:ARG:HH21	1.71	0.54
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.30	0.54
1:A:3648:VAL:HG22	1:A:3662:ILE:HD11	1.90	0.54
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.89	0.53
1:A:3233:ASN:OD1	1:A:3234:ALA:N	2.42	0.53
1:A:3977:GLU:OE2	1:A:3977:GLU:N	2.40	0.53
1:A:4195:ARG:HH11	1:A:4195:ARG:HG3	1.72	0.53
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.09	0.52
1:A:2075:LEU:HD22	1:A:4522:THR:HG23	1.91	0.52
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.40	0.52
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.91	0.52
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.91	0.52
1:A:1910:THR:HG21	1:A:2041:MET:O	2.10	0.52
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.90	0.52
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.92	0.52
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.49	0.52
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.91	0.52
1:A:3756:VAL:HG23	1:A:3766:ILE:HG13	1.91	0.52
1:A:4409:LEU:HD11	1:A:4558:PHE:HE2	1.75	0.52
1:A:2838:VAL:HG22	1:A:3093:TRP:CE2	2.45	0.52
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.36	0.51
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.91	0.51
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3653:VAL:HG11	1:A:3671:LEU:HD22	1.92	0.51
1:A:3217:GLU:HB2	1:A:3220:ARG:HH21	1.76	0.51
1:A:3969:THR:O	1:A:3969:THR:OG1	2.29	0.51
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.92	0.50
1:A:2454:CYS:HB3	1:A:2502:LEU:HD23	1.93	0.50
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	1.92	0.50
1:A:3601:MET:HE2	1:A:3611:ARG:HE	1.76	0.50
1:A:2792:TYR:OH	1:A:2842:GLU:OE1	2.26	0.50
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.94	0.50
1:A:1632:VAL:HG12	1:A:1656:LYS:HE3	1.93	0.50
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.26	0.50
1:A:3815:MET:HA	1:A:3818:LEU:HD12	1.94	0.50
1:A:4281:GLU:OE2	1:A:4281:GLU:N	2.44	0.50
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.93	0.50
1:A:1990:TYR:OH	1:A:1996:PRO:HA	2.12	0.49
1:A:2016:ILE:O	1:A:2016:ILE:HG13	2.12	0.49
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.93	0.49
1:A:2366:GLU:OE1	1:A:2451:ARG:NH2	2.45	0.49
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.25	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.93	0.49
1:A:3115:LEU:HD12	1:A:3143:ILE:HG13	1.93	0.49
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	1.93	0.49
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.24	0.49
1:A:4027:LEU:HD11	1:A:4043:MET:HE1	1.94	0.49
1:A:4027:LEU:HB3	1:A:4058:LEU:HD22	1.95	0.49
1:A:3939:SER:HA	1:A:3944:PHE:O	2.13	0.49
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.95	0.49
1:A:3584:ASN:O	1:A:3651:ARG:NH2	2.45	0.49
1:A:2671:MET:HG3	1:A:2677:GLN:HG3	1.93	0.48
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.95	0.48
1:A:2943:LYS:N	2:A:4704:ADP:O1B	2.46	0.48
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.96	0.48
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.47	0.48
1:A:4423:LEU:HD22	1:A:4466:HIS:HB2	1.95	0.48
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.53	0.48
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.96	0.48
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.95	0.48
1:A:4415:ARG:O	1:A:4419:MET:HG3	2.14	0.48
1:A:4554:ASP:OD1	1:A:4554:ASP:N	2.44	0.48
1:A:1635:GLU:HA	1:A:1638:LEU:HD12	1.95	0.48
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3902:ASP:OD1	1:A:3903:ALA:N	2.47	0.47
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.30	0.47
1:A:2369:LEU:O	1:A:2451:ARG:NH1	2.47	0.47
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.48	0.47
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.96	0.47
1:A:1999:CYS:SG	1:A:2001:LEU:HG	2.55	0.47
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.80	0.47
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.97	0.47
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.96	0.47
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.97	0.47
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.47	0.47
1:A:3211:THR:HG21	1:A:3760:ILE:HD12	1.97	0.47
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.47	0.47
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.95	0.47
1:A:4287:LYS:HA	1:A:4287:LYS:HD3	1.64	0.47
1:A:4448:LEU:HD23	1:A:4448:LEU:HA	1.79	0.47
1:A:2606:PHE:HE1	1:A:2617:VAL:HG21	1.80	0.47
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.97	0.47
1:A:3043:MET:O	1:A:3044:LEU:HD23	2.14	0.47
1:A:3478:LEU:HD11	1:A:3767:ILE:HG12	1.97	0.47
1:A:4157:MET:HE1	1:A:4308:TRP:HZ3	1.79	0.47
1:A:2138:ILE:HG12	1:A:2161:LEU:HD22	1.96	0.46
1:A:3945:LYS:HG3	1:A:3946:ASP:N	2.31	0.46
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.28	0.46
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.96	0.46
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.97	0.46
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.46	0.46
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	1.98	0.46
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.97	0.46
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.96	0.46
1:A:4378:ARG:HA	1:A:4378:ARG:HD3	1.73	0.46
1:A:2963:VAL:HG13	1:A:3000:LEU:HD11	1.97	0.45
1:A:2481:MET:SD	1:A:2485:GLN:HG2	2.56	0.45
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.98	0.45
1:A:2753:ARG:O	1:A:2763:ARG:NH1	2.49	0.45
1:A:2905:LEU:HD22	1:A:2907:VAL:HG13	1.98	0.45
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.15	0.45
1:A:3811:ILE:O	1:A:3815:MET:HG3	2.16	0.45
1:A:2601:LYS:NZ	2:A:4703:ADP:O3B	2.37	0.45
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.50	0.45
1:A:4489:LEU:HD11	1:A:4515:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2721:LYS:HB2	1:A:2721:LYS:HE2	1.84	0.45
1:A:2903:GLU:O	1:A:3654:ARG:NH2	2.42	0.45
1:A:4243:LEU:O	1:A:4247:MET:HG3	2.16	0.45
1:A:2865:LYS:HB2	1:A:2865:LYS:HE2	1.70	0.45
1:A:2536:ASP:OD2	1:A:2572:LEU:HD21	2.16	0.45
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.99	0.44
1:A:3941:LEU:HD12	1:A:3941:LEU:H	1.83	0.44
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	2.00	0.44
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.16	0.44
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.98	0.44
1:A:3731:LEU:HD21	1:A:3790:VAL:HG13	1.99	0.44
1:A:3169:MET:HA	1:A:3169:MET:HE2	1.99	0.44
1:A:3160:ARG:HG3	1:A:3160:ARG:HH11	1.83	0.44
1:A:3171:ILE:HD13	1:A:3171:ILE:HA	1.89	0.44
1:A:3581:LYS:HE2	1:A:3581:LYS:HB3	1.83	0.43
1:A:1665:ILE:HG22	1:A:1674:LEU:HB2	2.00	0.43
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.76	0.43
1:A:1933:ASP:OD1	1:A:1935:THR:HG22	2.19	0.43
1:A:4258:ASN:OD1	1:A:4259:GLU:N	2.51	0.43
1:A:3741:ARG:HA	1:A:3741:ARG:HD2	1.77	0.43
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	2.00	0.43
1:A:3109:PHE:HB3	1:A:3180:ILE:HG21	1.99	0.43
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.92	0.43
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	2.01	0.43
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.84	0.43
1:A:3088:ARG:HA	1:A:3088:ARG:HD3	1.81	0.43
1:A:3734:LEU:HD12	1:A:3734:LEU:HA	1.92	0.43
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.52	0.43
1:A:1672:VAL:HG12	1:A:1674:LEU:HD23	1.99	0.43
1:A:2506:SER:HB2	1:A:2510:MET:HB2	2.00	0.43
1:A:2571:THR:H	1:A:2574:THR:HB	1.84	0.43
1:A:4535:SER:OG	1:A:4537:GLU:OE1	2.30	0.43
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.54	0.43
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	2.01	0.43
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	2.01	0.43
1:A:2816:LEU:HD21	1:A:2821:LEU:N	2.34	0.43
1:A:3157:ALA:HB1	1:A:3524:MET:HE3	2.01	0.42
1:A:3872:ALA:HA	1:A:3875:MET:HB2	2.00	0.42
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	2.00	0.42
1:A:2256:PRO:HD2	1:A:2305:GLY:HA3	2.01	0.42
1:A:3073:GLU:OE1	1:A:3073:GLU:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1647:VAL:HG21	1:A:1666:LEU:HD22	2.01	0.42
1:A:1695:HIS:HA	1:A:1697:LYS:NZ	2.34	0.42
1:A:3868:PHE:CZ	1:A:4018:MET:HG2	2.54	0.42
1:A:4413:PHE:CD2	1:A:4504:LEU:HD22	2.54	0.42
1:A:1694:GLU:OE1	1:A:1694:GLU:N	2.52	0.42
1:A:1882:THR:HB	1:A:2045:ASP:HB2	2.01	0.42
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	2.01	0.42
1:A:3003:GLY:O	1:A:3007:ARG:HG3	2.20	0.42
1:A:3163:LYS:HA	1:A:3163:LYS:HD3	1.88	0.42
1:A:4089:LYS:HB2	1:A:4089:LYS:HE3	1.71	0.42
1:A:1672:VAL:HG22	1:A:1691:SER:HB3	2.01	0.42
1:A:2017:THR:O	1:A:2018:MET:HG3	2.19	0.42
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.55	0.42
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.53	0.42
1:A:3907:HIS:CE1	1:A:3938:LEU:HA	2.54	0.42
1:A:4020:ILE:HG23	1:A:4021:MET:SD	2.59	0.42
1:A:1878:LYS:HE2	1:A:1878:LYS:HB3	1.85	0.42
1:A:1961:ASN:OD1	1:A:1961:ASN:N	2.49	0.42
1:A:2485:GLN:NE2	1:A:2542:SER:O	2.41	0.42
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.55	0.42
1:A:2847:ASP:OD1	1:A:2869:ARG:NH1	2.52	0.42
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.85	0.42
1:A:2313:GLU:OE2	1:A:2355:THR:OG1	2.37	0.42
1:A:1960:PHE:HE2	1:A:2032:LEU:HD21	1.84	0.41
1:A:2633:LYS:HD3	1:A:2633:LYS:HA	1.75	0.41
1:A:4150:PRO:HG2	1:A:4156:ASN:HA	2.01	0.41
1:A:4465:SER:O	1:A:4465:SER:OG	2.37	0.41
1:A:2176:THR:O	1:A:2180:GLU:HG2	2.20	0.41
1:A:2388:ASP:OD2	1:A:2389:GLU:N	2.53	0.41
1:A:4629:LYS:HD3	1:A:4629:LYS:C	2.45	0.41
1:A:1797:LEU:HD23	1:A:1797:LEU:HA	1.93	0.41
1:A:1990:TYR:HE1	1:A:1995:ALA:O	2.03	0.41
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.20	0.41
1:A:4394:THR:O	1:A:4490:GLN:NE2	2.53	0.41
1:A:1638:LEU:HA	1:A:1641:ILE:HD12	2.01	0.41
1:A:1640:ILE:CG2	1:A:1698:ILE:HG12	2.51	0.41
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.41
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.20	0.41
1:A:2221:MET:SD	1:A:2361:MET:HE1	2.61	0.41
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.55	0.41
1:A:1943:ARG:HH12	1:A:2273:ARG:NE	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2322:ASN:O	1:A:2323:LYS:C	2.63	0.41
1:A:2483:ILE:HD12	1:A:2483:ILE:HA	1.97	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.55	0.41
1:A:1891:THR:HB	1:A:2039:LEU:HD22	2.02	0.41
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	2.02	0.41
1:A:3776:GLU:HA	1:A:3779:GLU:HG2	2.02	0.41
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.21	0.41
1:A:2642:ARG:HH12	1:A:2651:ALA:HB3	1.85	0.41
1:A:4312:LEU:HD23	1:A:4312:LEU:HA	1.89	0.41
1:A:2047:GLN:NE2	1:A:2067:ASN:OD1	2.54	0.41
1:A:2864:GLU:HG2	1:A:2865:LYS:N	2.35	0.41
1:A:2936:ILE:HD12	1:A:3091:LEU:HD21	2.02	0.41
1:A:3077:ASP:O	1:A:3081:THR:HG22	2.21	0.41
1:A:3126:MET:HE3	1:A:3127:PRO:HD2	2.03	0.41
1:A:3950:LYS:HB3	1:A:3973:LEU:HD22	2.01	0.41
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.03	0.41
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	2.02	0.41
1:A:1543:ARG:HB3	1:A:1608:LEU:HD12	2.04	0.41
1:A:1628:ARG:NE	1:A:1706:GLU:OE2	2.52	0.41
1:A:1769:MET:HG3	1:A:1777:PRO:HD2	2.01	0.40
1:A:2822:ILE:HD11	1:A:2858:PHE:CD1	2.56	0.40
1:A:3650:ASN:HD21	1:A:3695:ARG:NH1	2.19	0.40
1:A:3846:LEU:HD22	1:A:3855:ARG:HG2	2.04	0.40
1:A:4183:LEU:HD12	1:A:4183:LEU:HA	1.82	0.40
1:A:2668:LEU:HD23	1:A:2668:LEU:HA	1.92	0.40
1:A:1904:PRO:HB2	1:A:1912:LYS:HG2	2.03	0.40
1:A:2018:MET:HE3	1:A:2018:MET:HB2	1.83	0.40
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.55	0.40
1:A:2004:LYS:HD2	1:A:2004:LYS:HA	1.78	0.40
1:A:1873:LEU:O	1:A:1876:GLN:NE2	2.54	0.40
1:A:2189:MET:HE3	1:A:2239:LYS:HE3	2.04	0.40
1:A:3207:LYS:O	1:A:3211:THR:HG23	2.22	0.40
1:A:4095:MET:HE3	1:A:4097:LYS:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2851/4646 (61%)	2809 (98%)	42 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	2532/4125 (61%)	2526 (100%)	6 (0%)	92 96

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

Mol	Chain	Res	Type
1	A	1690	VAL
1	A	1991	ASP
1	A	2138	ILE
1	A	2734	VAL
1	A	3875	MET
1	A	4127	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1559	HIS
1	A	1598	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1974	GLN
1	A	1976	GLN
1	A	2005	GLN
1	A	2217	ASN
1	A	2677	GLN
1	A	2698	GLN
1	A	3214	GLN
1	A	3535	HIS
1	A	3563	GLN
1	A	3711	GLN
1	A	3754	ASN
1	A	3877	HIS
1	A	3952	GLN
1	A	4029	HIS
1	A	4114	HIS
1	A	4335	GLN
1	A	4508	HIS
1	A	4566	GLN
1	A	4595	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
2	ADP	A	4703	-	24,29,29	0.89	0	29,45,45	1.23	2 (6%)
2	ADP	A	4701	-	24,29,29	0.73	0	29,45,45	0.78	1 (3%)
3	ATP	A	4702	4	28,33,33	0.75	0	34,52,52	0.80	1 (2%)
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.18	2 (6%)

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
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	0/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	0/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4703	ADP	N3-C2-N1	-3.69	123.66	128.67
2	A	4704	ADP	N3-C2-N1	-3.56	123.83	128.67
2	A	4704	ADP	C4-C5-N7	-2.55	106.64	109.34
2	A	4703	ADP	C4-C5-N7	-2.47	106.72	109.34
3	A	4702	ATP	C5-C6-N6	2.34	123.88	120.31
2	A	4701	ADP	C5-C6-N6	2.26	123.76	120.31

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4703	ADP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A

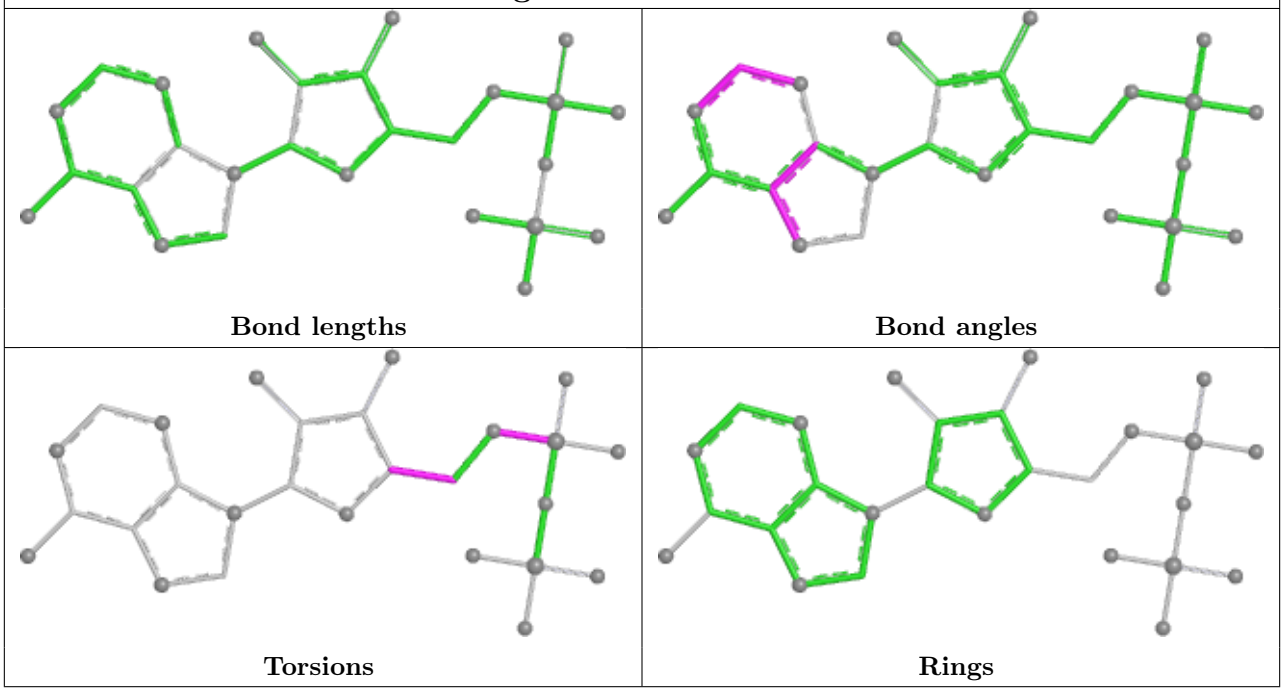
There are no ring outliers.

3 monomers are involved in 3 short contacts:

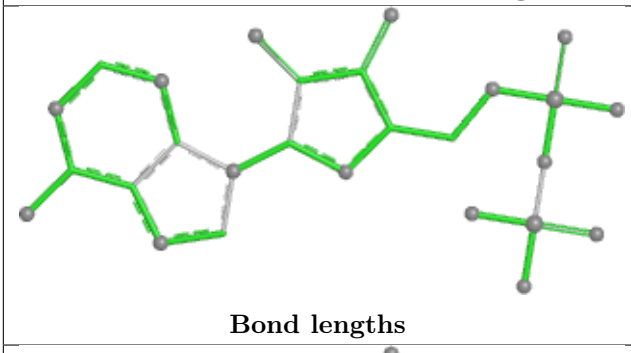
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4703	ADP	1	0
2	A	4701	ADP	1	0
2	A	4704	ADP	1	0

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.

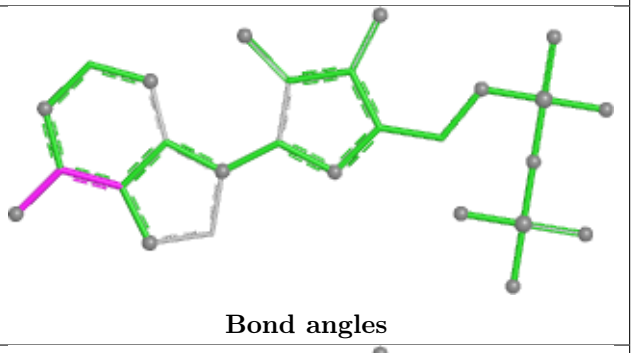
Ligand ADP A 4703



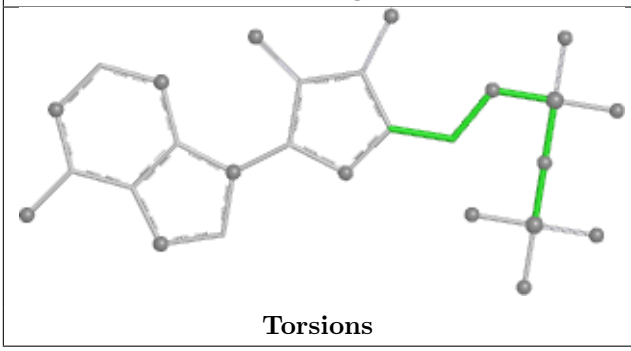
Ligand ADP A 4701



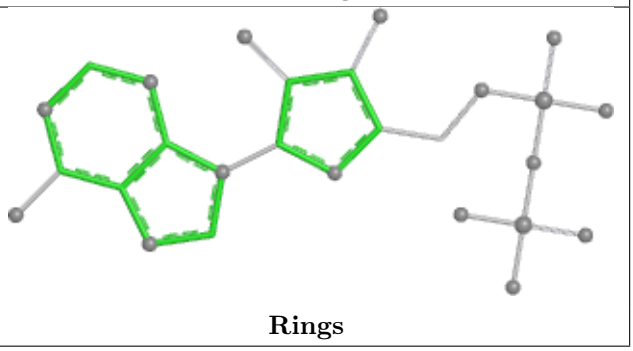
Bond lengths



Bond angles

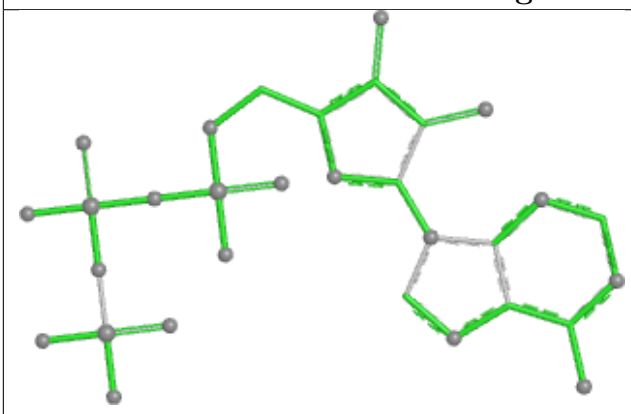


Torsions

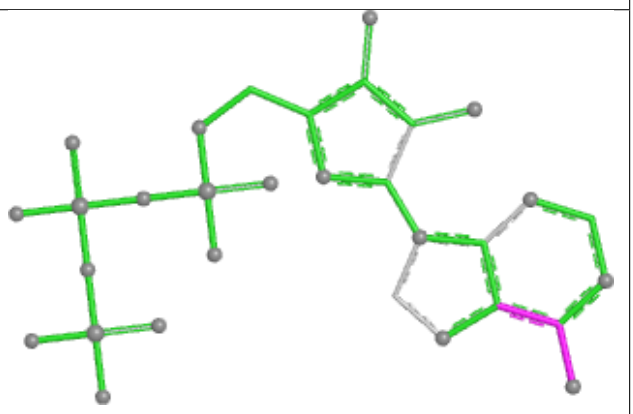


Rings

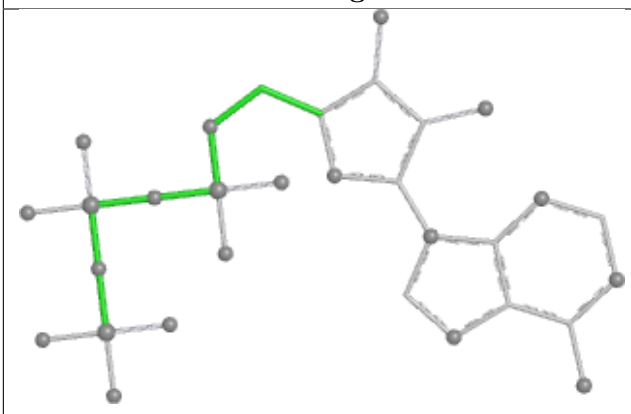
Ligand ATP A 4702



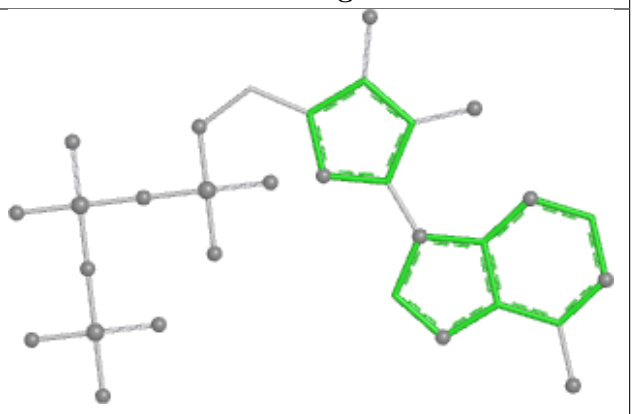
Bond lengths



Bond angles

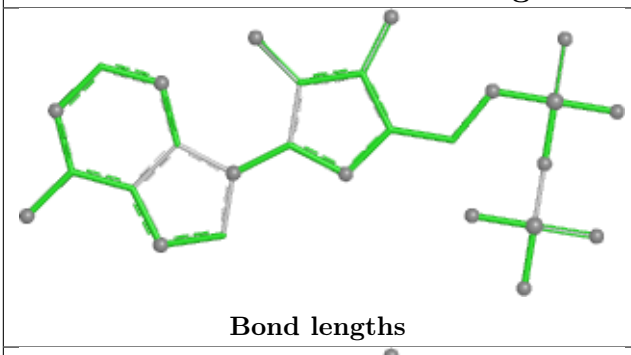


Torsions

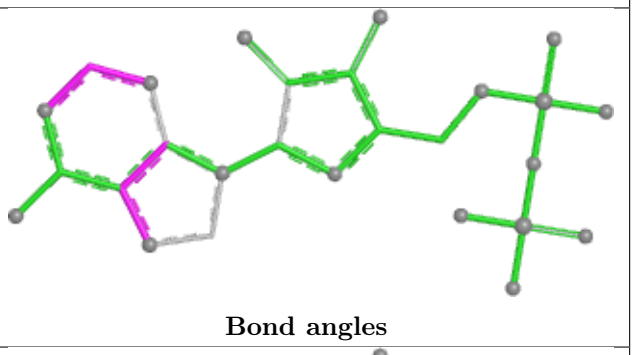


Rings

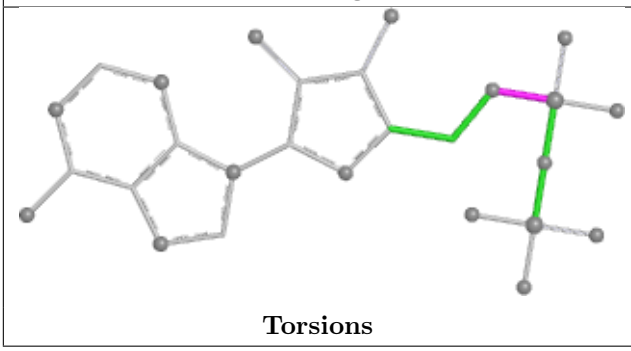
Ligand ADP A 4704



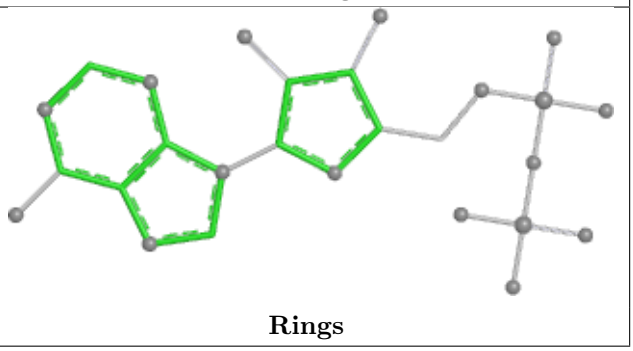
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

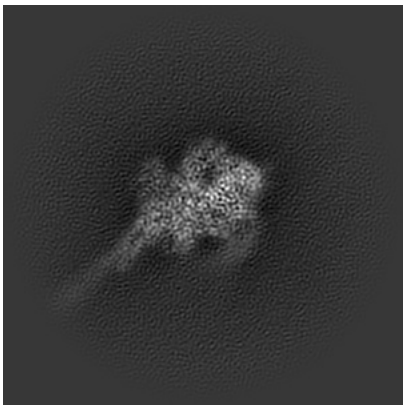
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44703. These allow visual inspection of the internal detail of the map and identification of artifacts.

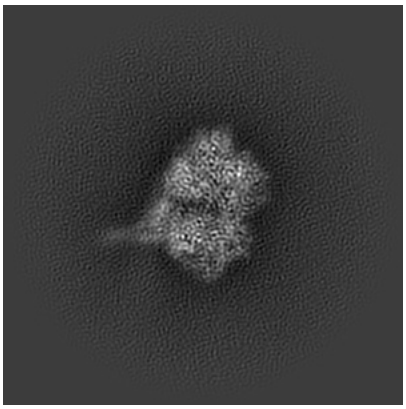
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

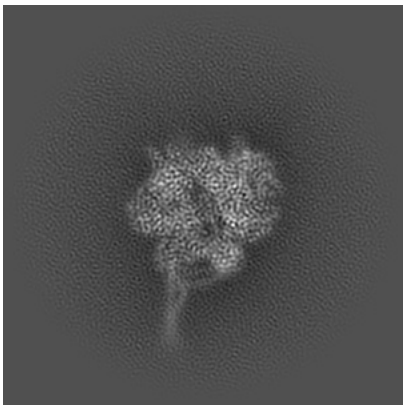
6.1.1 Primary map



X

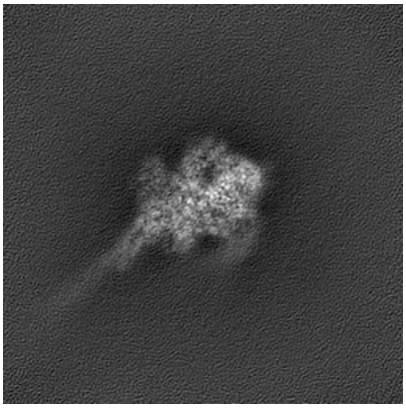


Y

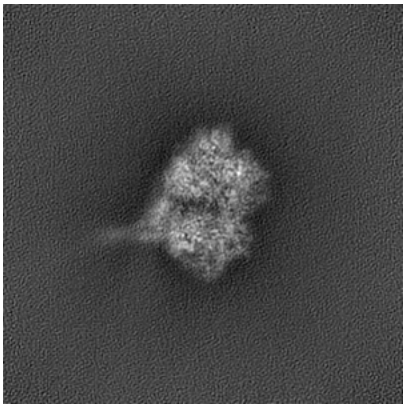


Z

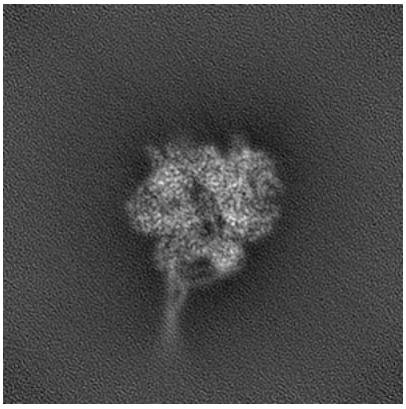
6.1.2 Raw map



X



Y

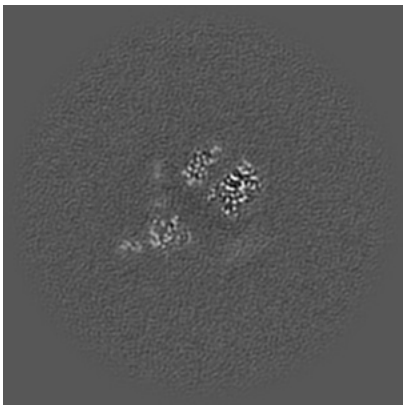


Z

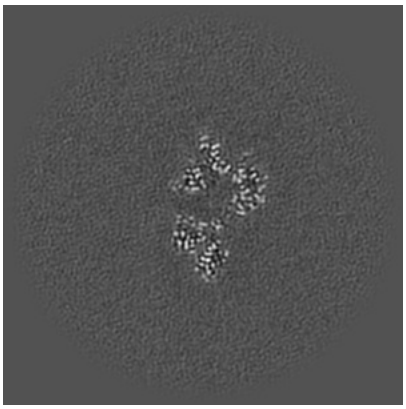
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

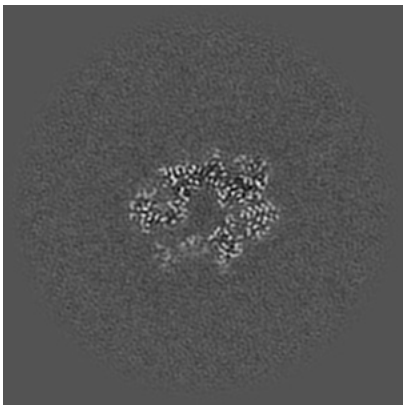
6.2.1 Primary map



X Index: 128

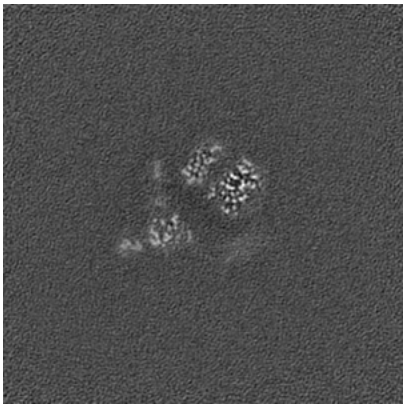


Y Index: 128

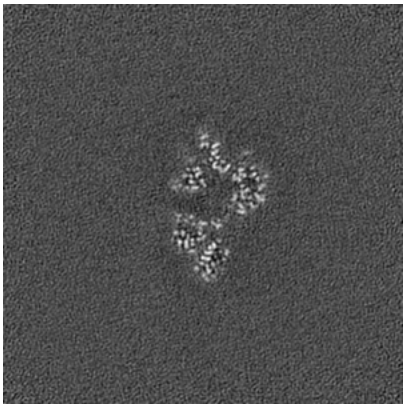


Z Index: 128

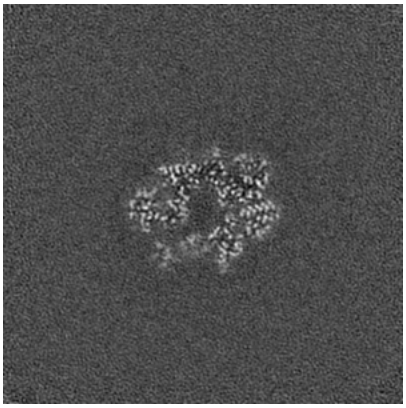
6.2.2 Raw map



X Index: 128



Y Index: 128

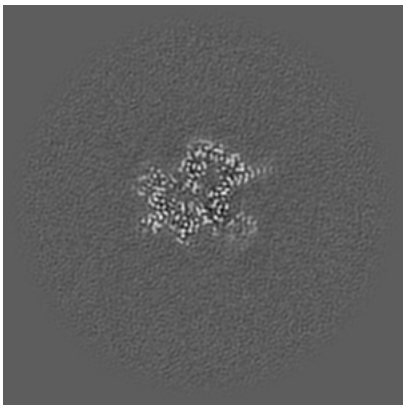


Z Index: 128

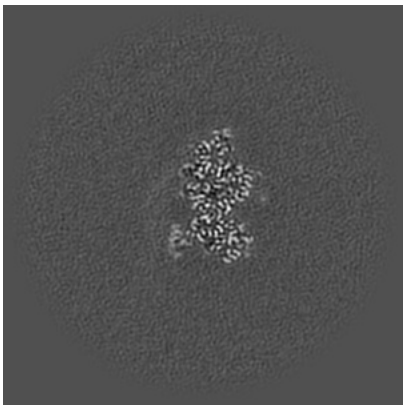
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

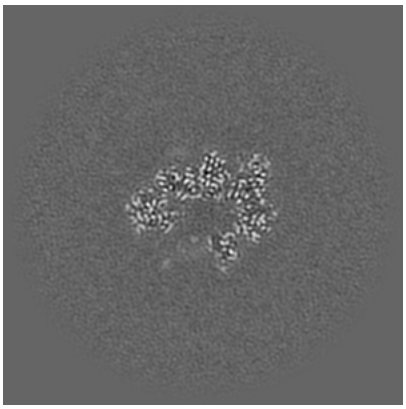
6.3.1 Primary map



X Index: 146

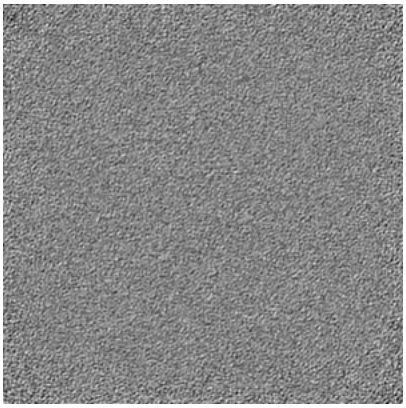


Y Index: 143

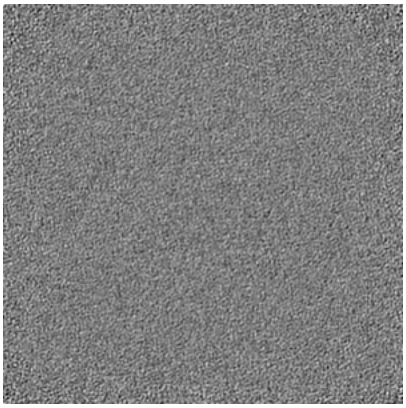


Z Index: 131

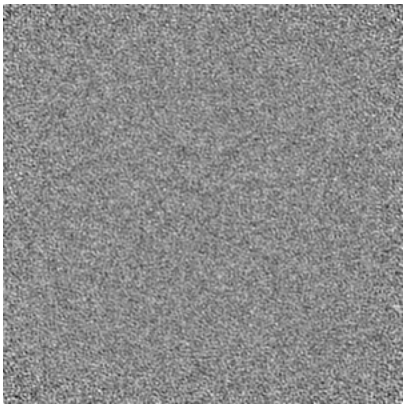
6.3.2 Raw map



X Index: 0



Y Index: 0

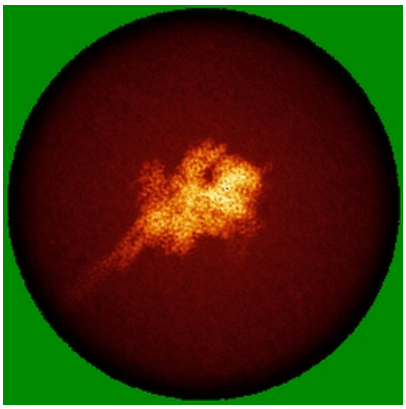


Z Index: 0

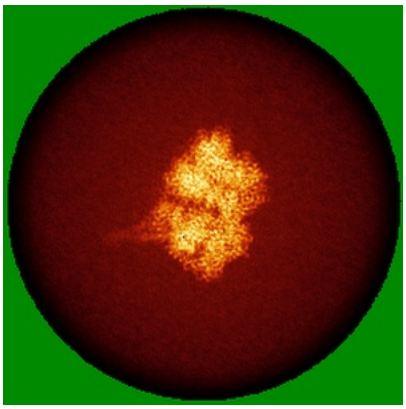
The images above show the largest variance slices of the map in three orthogonal directions.

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

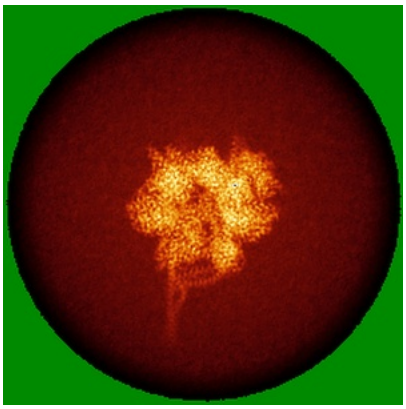
6.4.1 Primary map



X

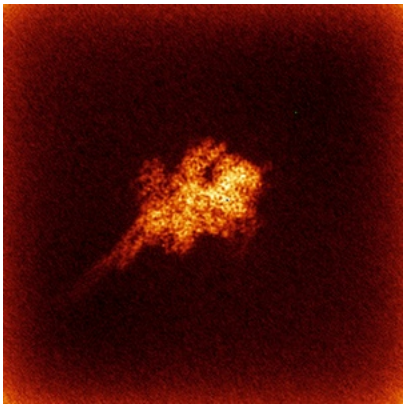


Y

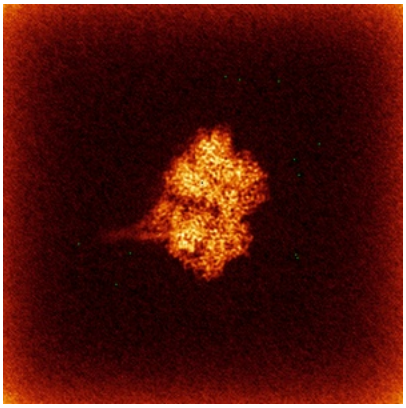


Z

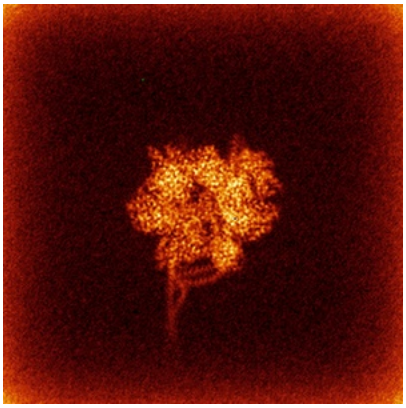
6.4.2 Raw map



X



Y

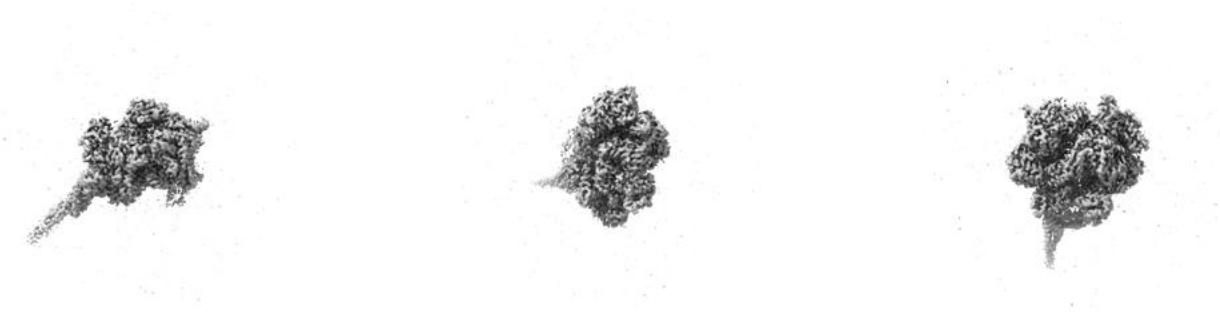


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

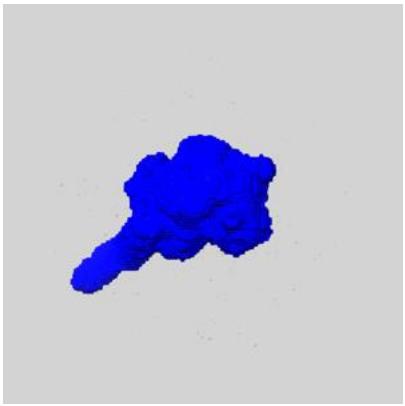
6.6 Mask visualisation (i)

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

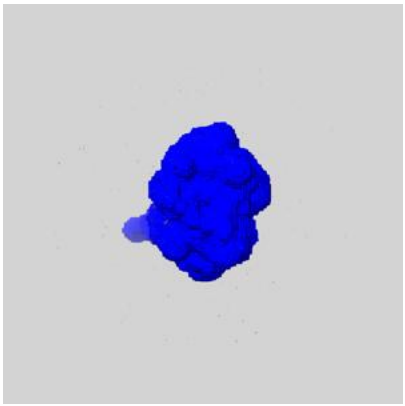
A mask typically either:

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

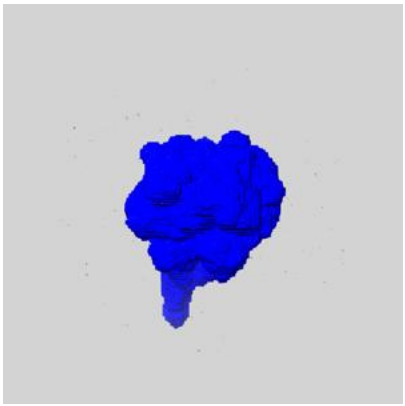
6.6.1 emd_44703_msk_1.map (i)



X



Y

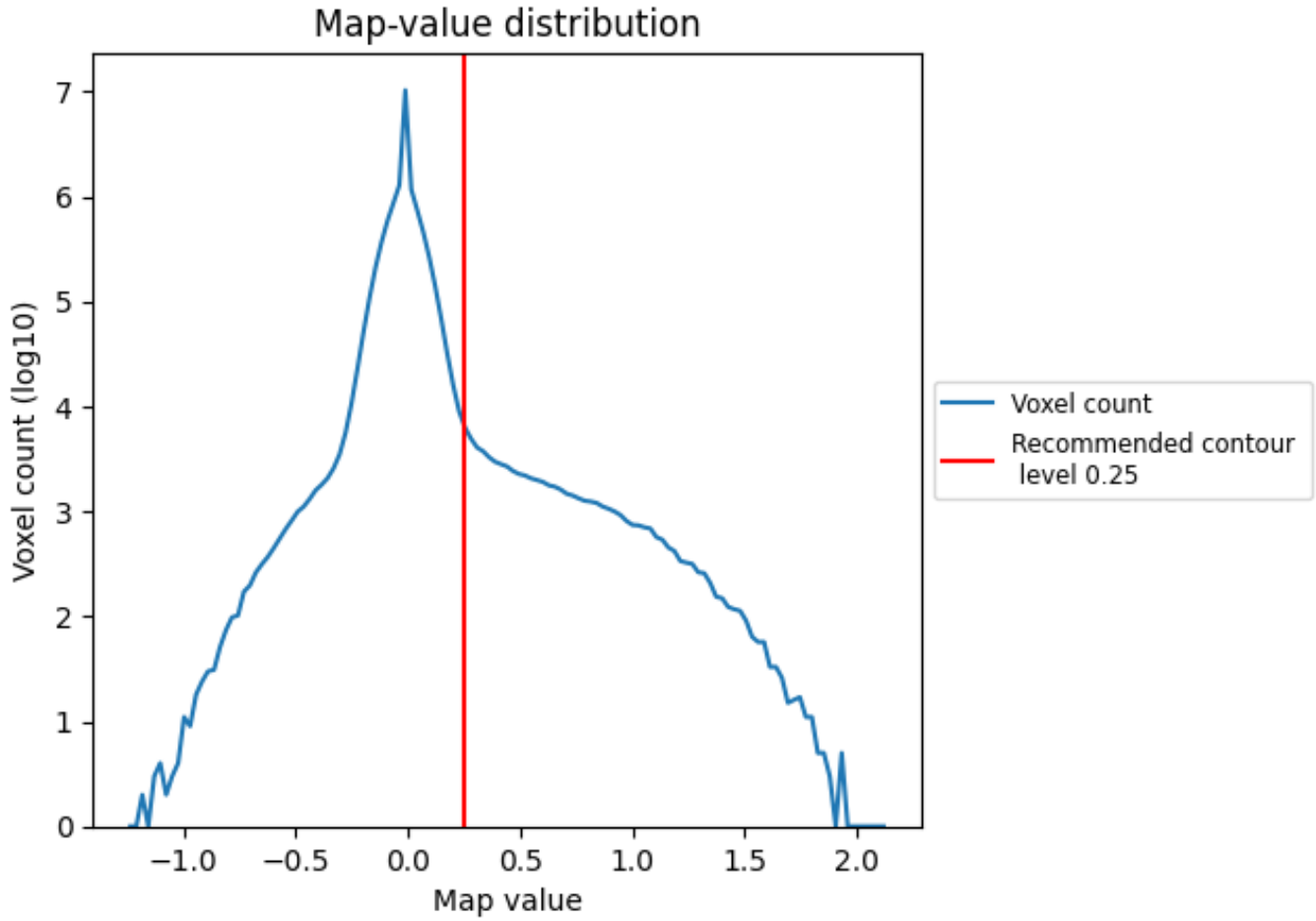


Z

7 Map analysis

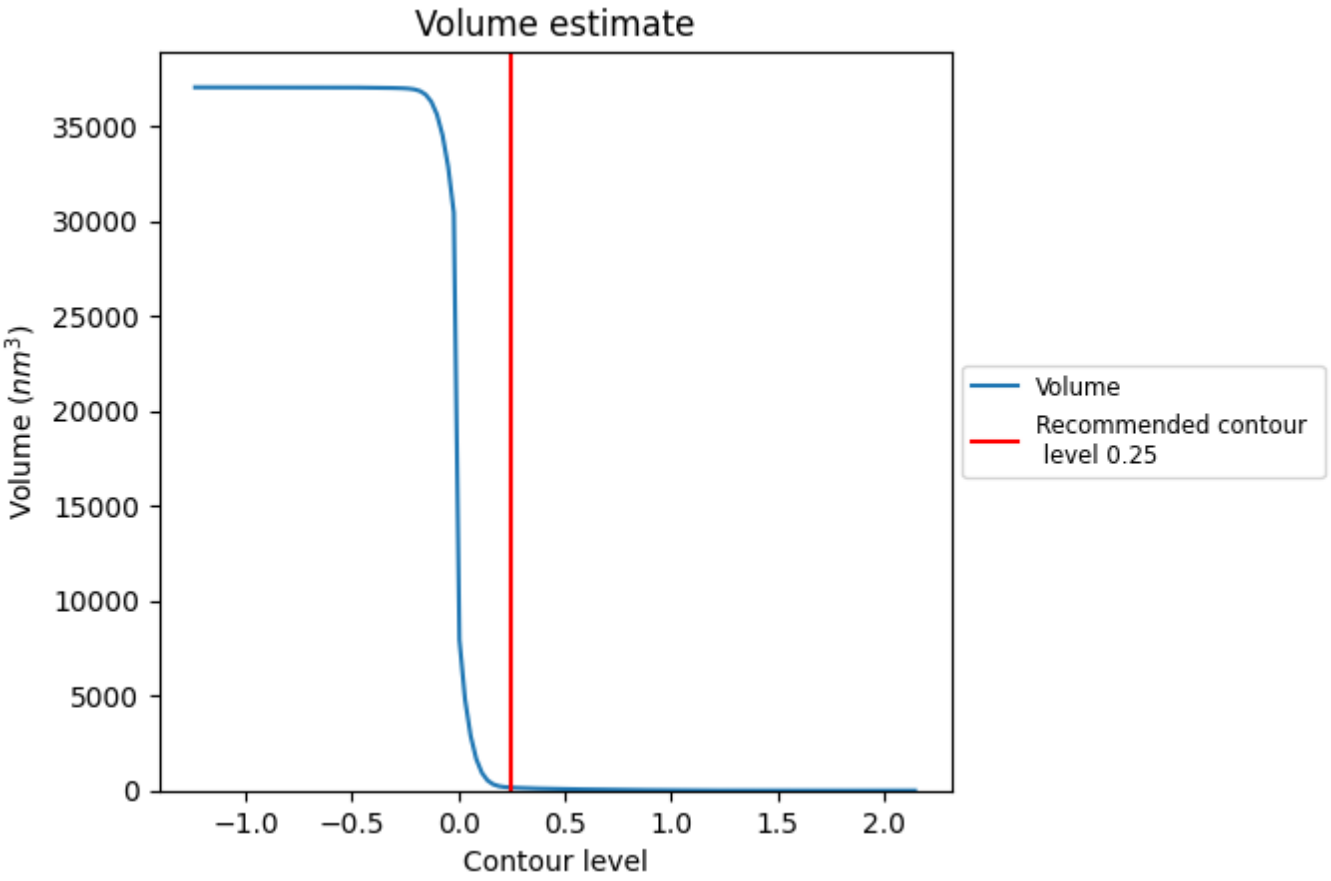
This section contains the results of statistical analysis of the map.

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.

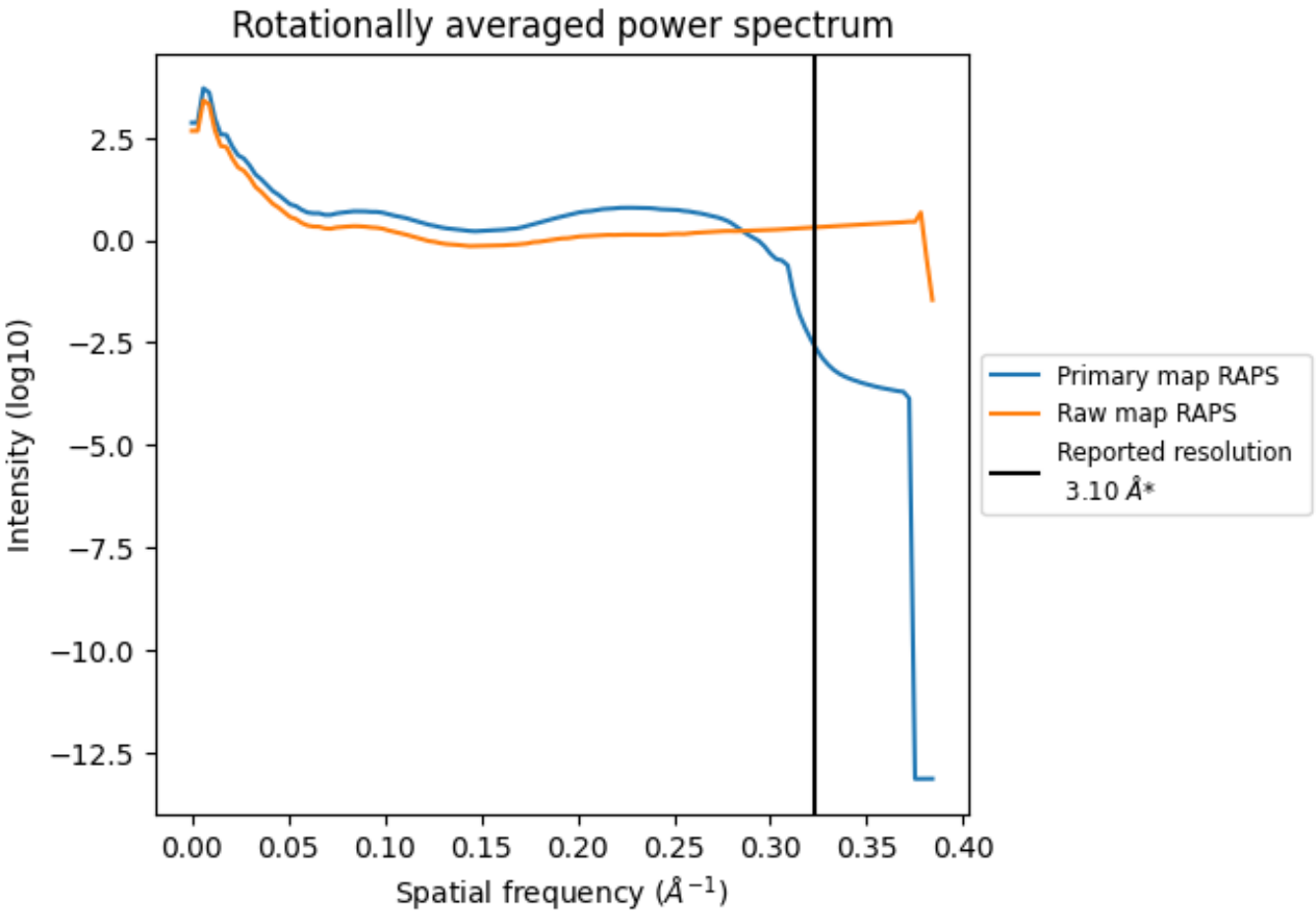
7.2 Volume estimate



The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 141 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)

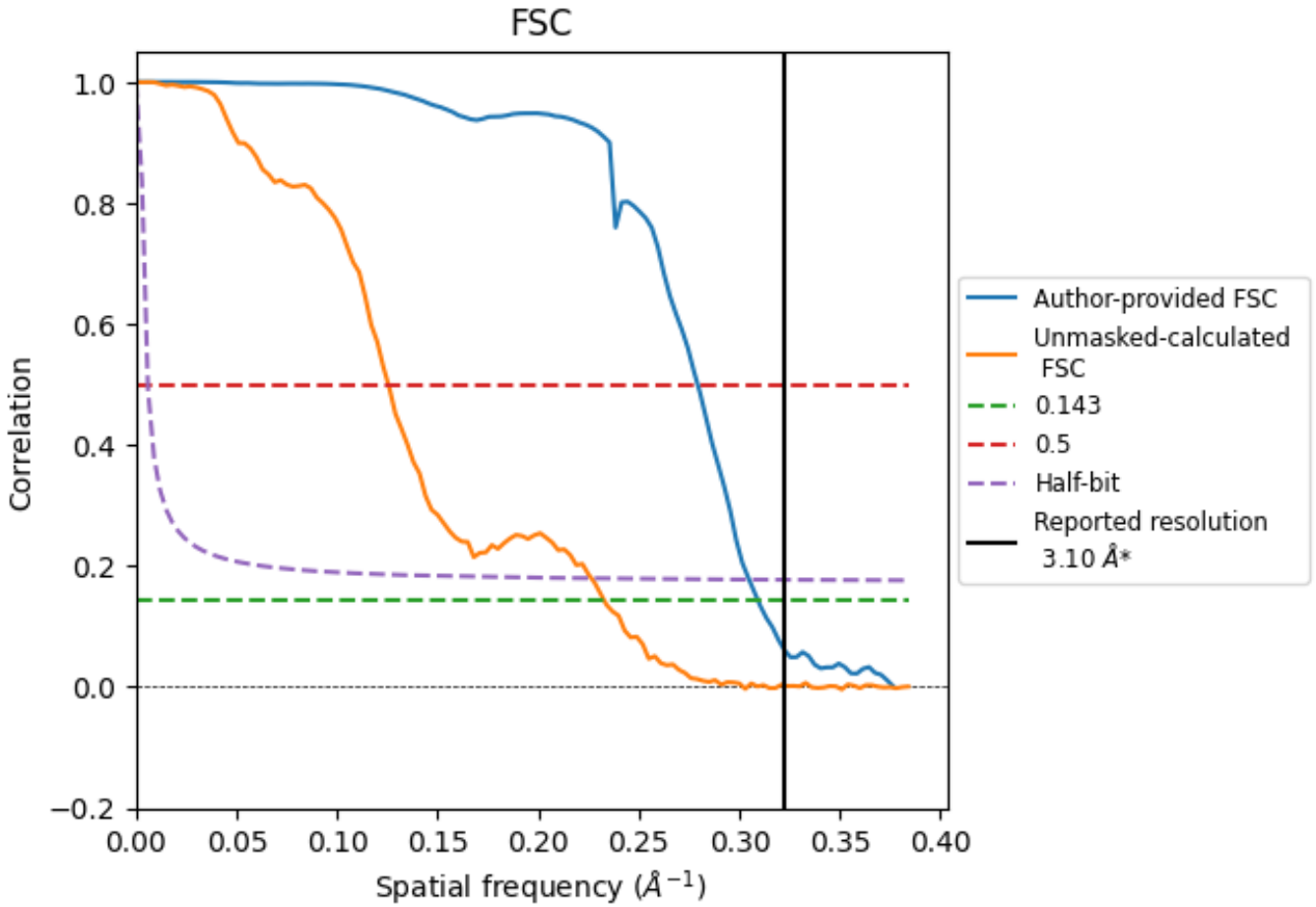


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

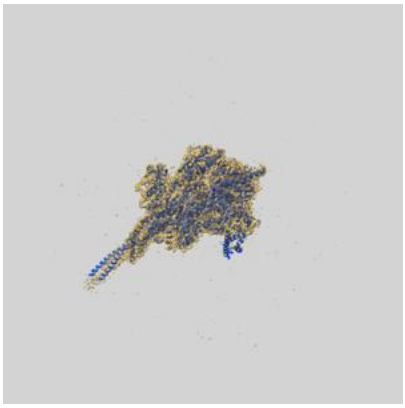
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.23	3.58	3.28
Unmasked-calculated*	4.30	7.97	4.42

*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 4.30 differs from the reported value 3.1 by more than 10 %

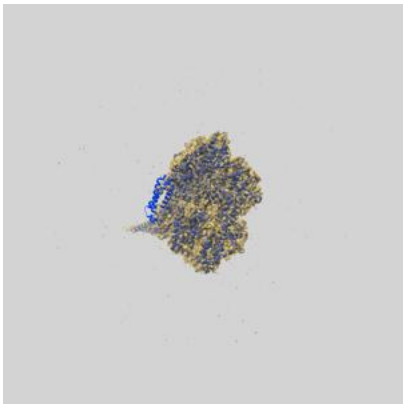
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44703 and PDB model 9BMM. Per-residue inclusion information can be found in section 3 on page 5.

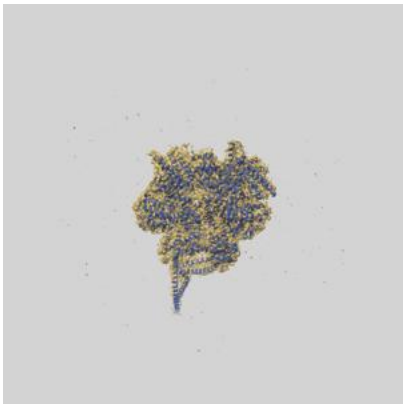
9.1 Map-model overlay



X



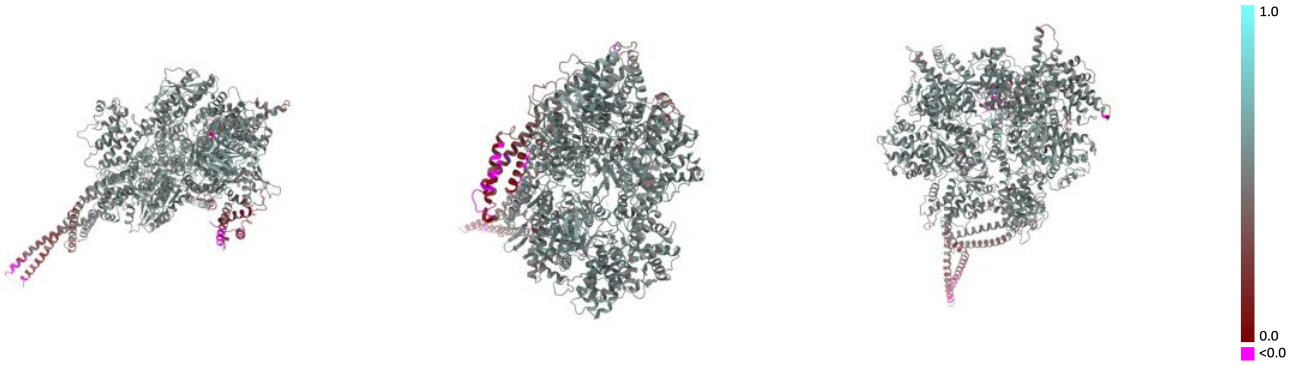
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

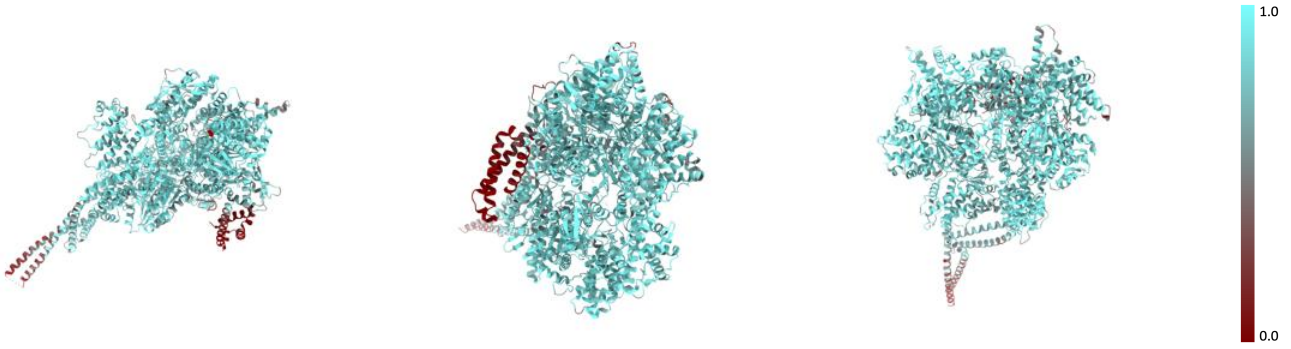
9.2 Q-score mapped to coordinate model (i)



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.

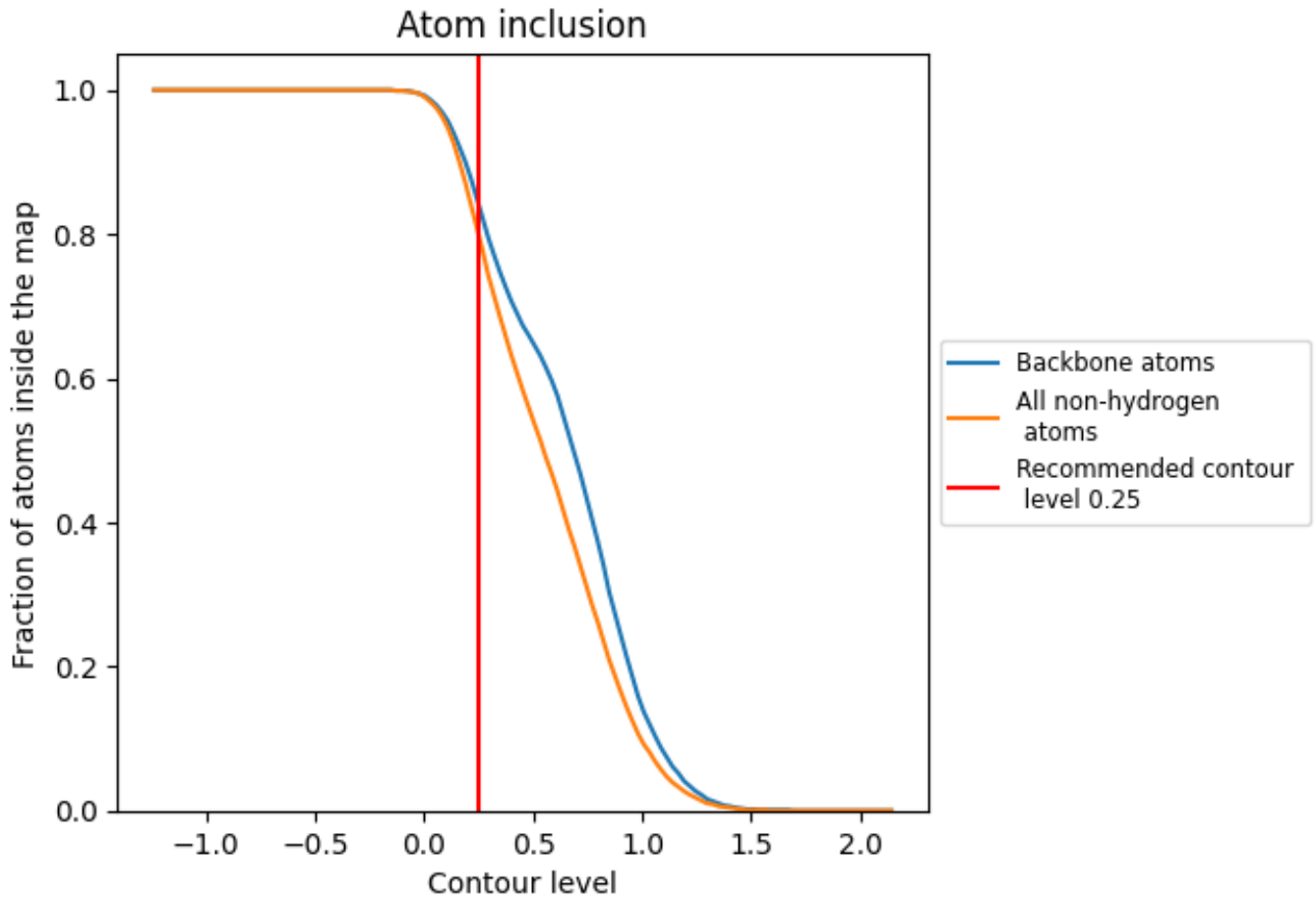
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.4970
A	0.8000	0.4970