Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 03:46 PM EDT

PDB ID	:	9DH7 / pdb_00009dh7
EMDB ID	:	EMD-46858
Title	:	State-4 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg2+
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-09-03
Resolution	:	3.40 Å(reported)

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

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

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

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

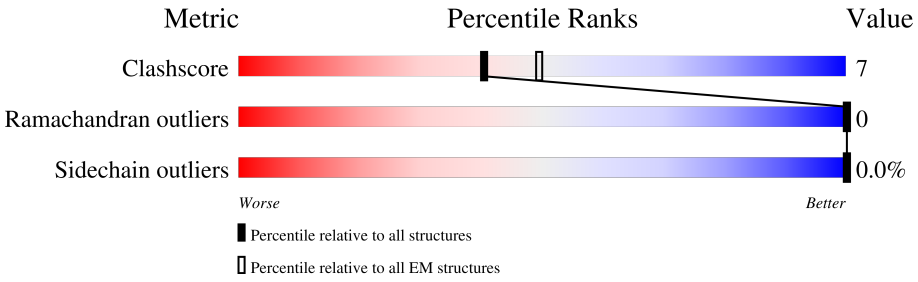
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition

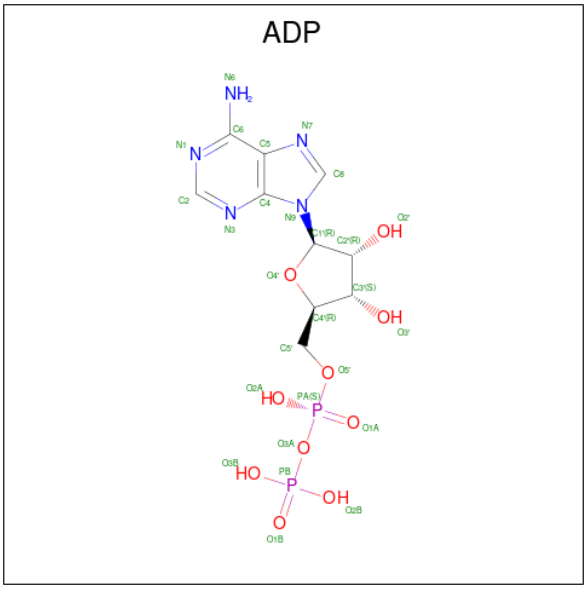
There are 4 unique types of molecules in this entry. The entry contains 23020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

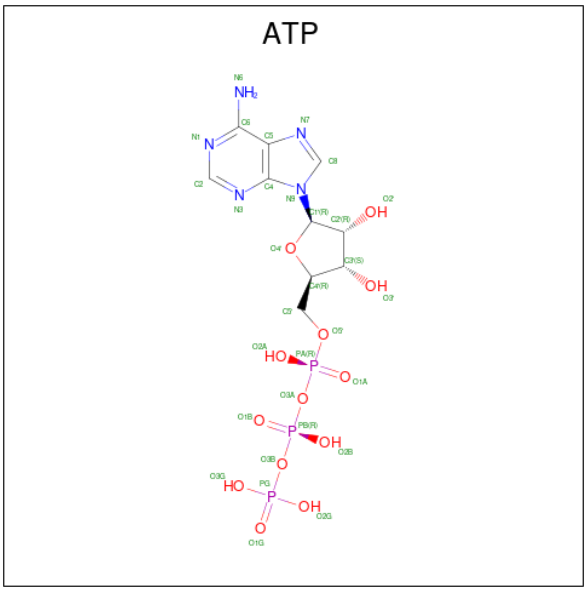
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2857	22907	14584	3957	4253	113	0	0

- 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).

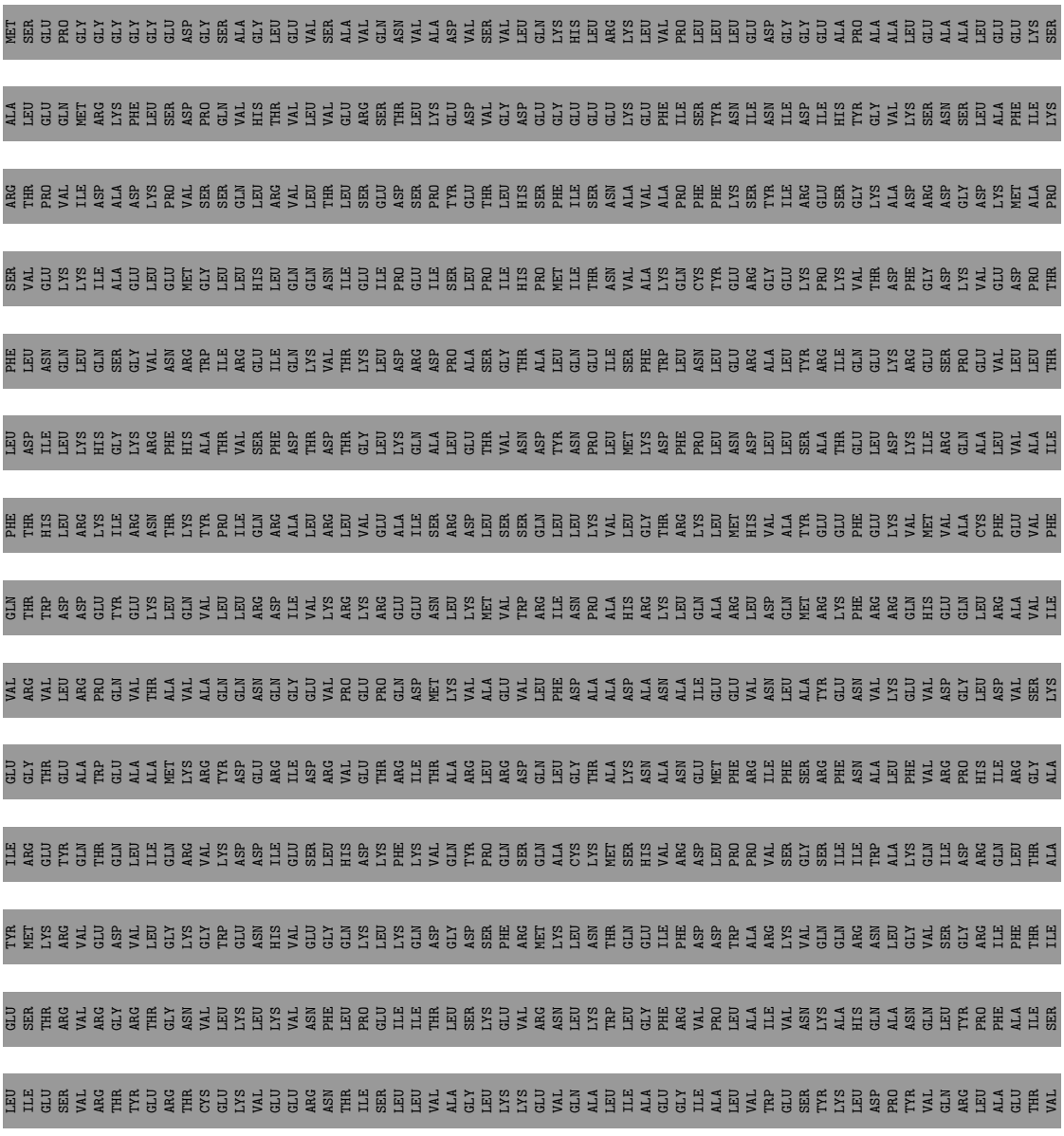
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

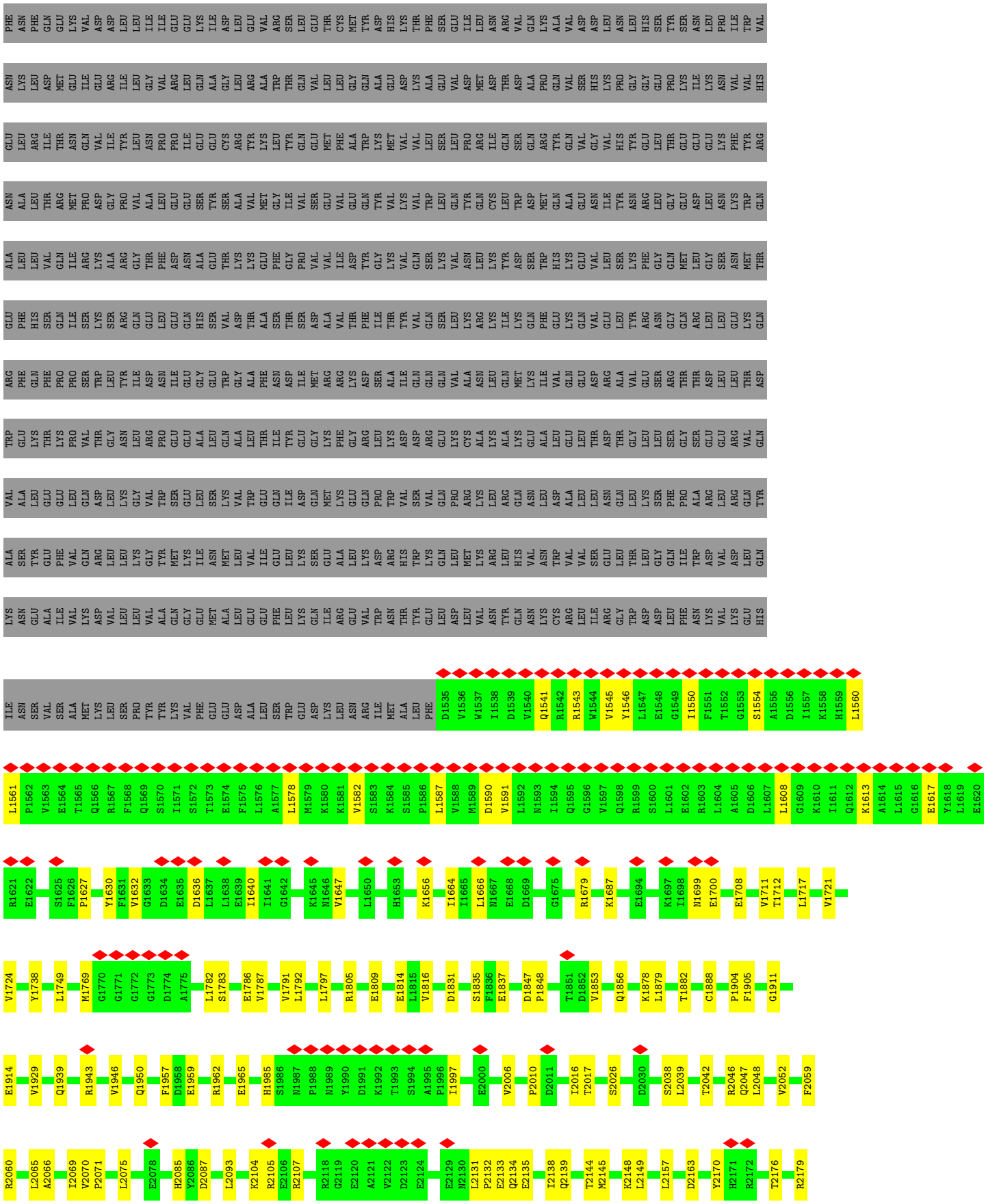
3 Residue-property plots (i)

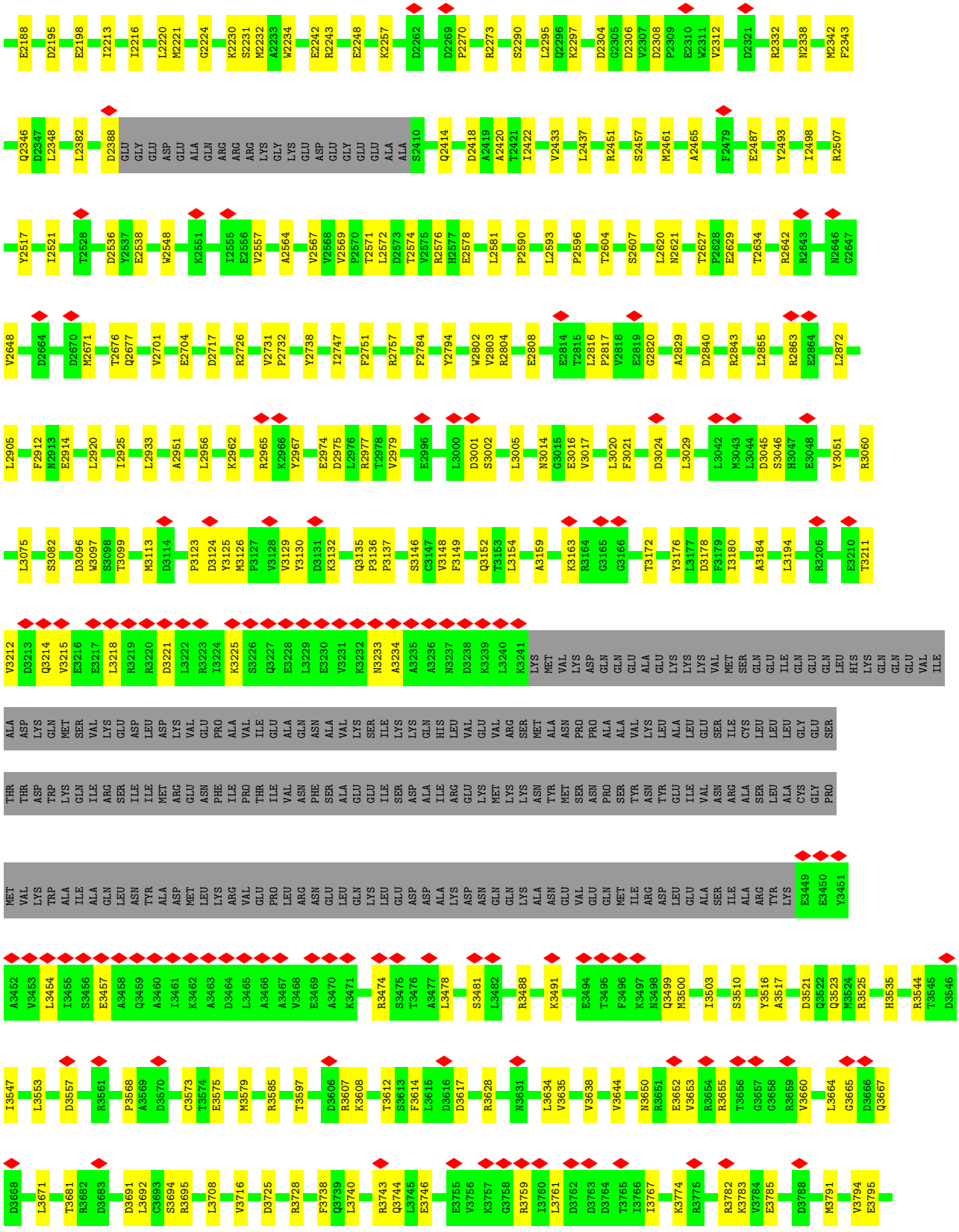
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

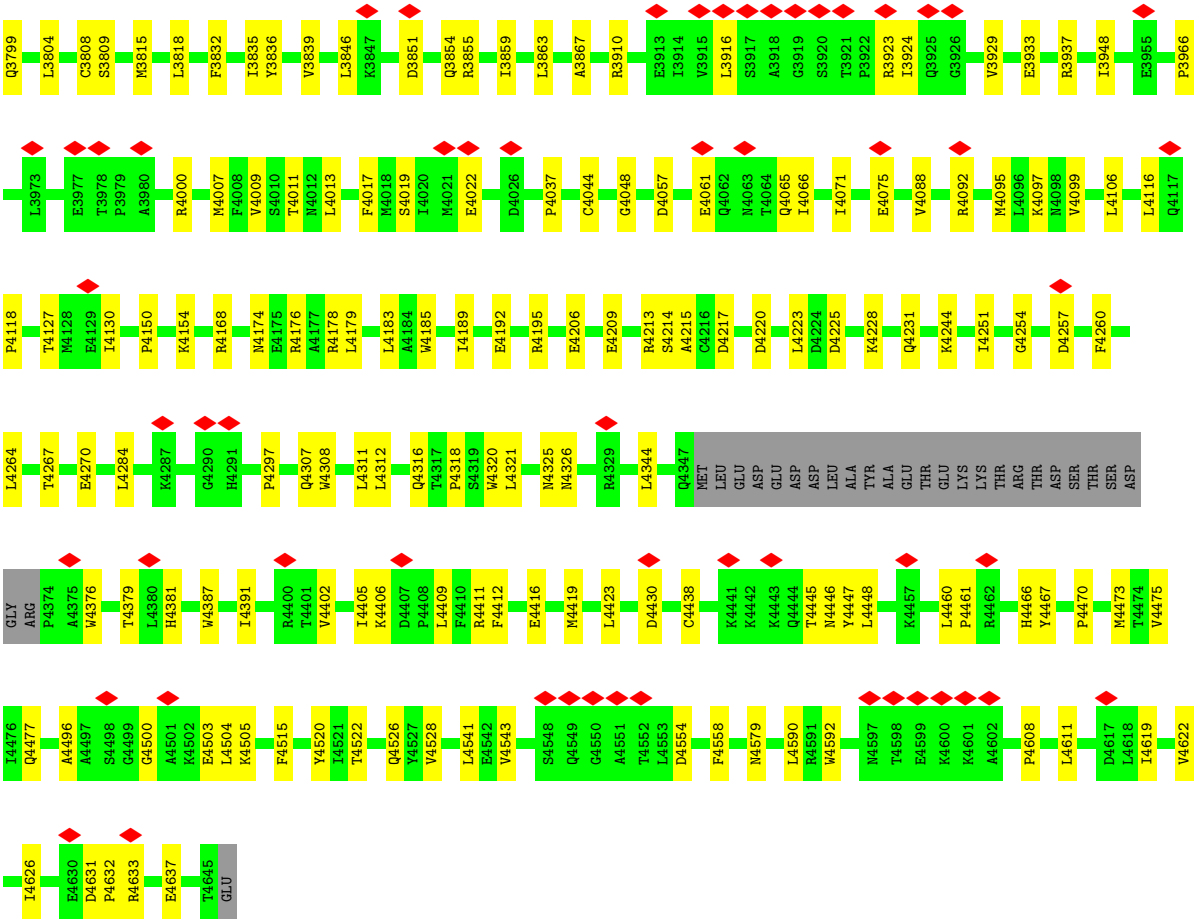
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

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 VAL HIS
ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ARG LEU GLN ALA GLY LEU ARG ALA TRP THR GLN VAL LEU LEU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP MET ASP THR ASP ALA PRO GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS
GLU LEU ARG ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU GLU SER LEU PRO ARG GLN ILE GLN SER GLU GLU GLY GLU LYS PHE TYR ARG
ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER TYR SER ALA VAL MET GLY ILE VAL SER GLU VAL GLN TYR GLN CYS LEU TRP ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS 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 TYR GLN PHE GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN GLU LEU ARG LYS ASP GLN LEU LEU GLU LYS LYS
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ARG ARG LYS ASP SER ALA ILE ASP ASN LEU GLN MET LYS ILE VAL ASN LEU GLN ALA VAL GLU ASP ARG ALA VAL GLN GLU ASP ASP ARG THR THR ASP
TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN ALA LEU SER 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 SER
VAL ALA LEU GLU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU GLN 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 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 GLU ASP TRP ASP SER LYS VAL LYS 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 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 E1622 S1625 F1626 P1627 Y1630 F1631 V1632 G1633 D1634 E1635 D1636 L1637 L1638 E1639 I1640 I1641 G1642 K1645 N1646 V1647 L1650 H1653 K1656 I1664 I1665 L1666 N1667 E1668 D1669 G1675 R1679 K1687 E1694 K1697 I1698 N1699 E1700 E1708 V1711 T1712 L1717 V1721
V1724 Y1738 L1749 M1769 G1770 G1771 G1772 G1773 D1774 A1775 L1782 S1783 E1786 V1787 V1791 L1792 L1797 R1805 E1809 E1814 L1815 V1816 D1831 S1835 F1836 E1837 D1847 P1848 T1851 D1852 V1853 Q1856 K1878 L1879 T1882 C1888 P1904 F1905 G1911
E1914 V1929 Q1939 R1943 V1946 Q1950 F1957 D1958 E1959 R1962 E1965 H1985 S1986 N1987 P1988 N1989 Y1990 D1991 K1992 T1993 S1994 A1995 P1996 I1997 E2000 V2006 P2010 D2011 I2016 T2017 S2026 D2030 S2038 L2039 T2042 R2046 Q2047 L2048 V2052 F2059
R2060 L2065 A2066 I2069 V2070 P2071 L2075 E2078 H2085 Y2086 D2087 L2093 K2104 R2105 E2106 R2107 R2118 G2119 E2120 A2121 V2122 D2123 E2124 E2129 N2130 L2131 P2132 E2133 Q2134 E2135 I2138 Q2139 T2144 M2145 K2148 L2149 L2157 D2163 Y2170 H2171 R2172 T2176 R2179




Q3799 L3804 C3808 S3809 M3815 L3818 F3832 I3835 Y3836 V3839 L3846 K3847 D3851 Q3854 R3855 I3859 L3863 A3867 R3910 E3913 I3914 V3915 L3916 S3917 A3918 G3919 S3920 T3921 P3922 R3923 I3924 Q3925 G3926 V3929 E3933 R3937 I3948 E3965 P3966
L3973 E3977 T3978 P3979 A3980 R4000 M4007 F4008 V4009 S4010 T4011 N4012 L4013 F4017 M4018 S4019 I4020 M4021 E4022 D4026 P4037 C4044 G4048 D4057 E4061 Q4062 N4063 T4064 Q4065 I4066 I4071 E4075 V4088 R4092 M4095 L4096 K4097 N4098 V4099 L4106 L4116 Q4117
P4118 T4127 M4128 E4129 I4130 P4150 K4154 R4168 N4174 E4175 R4176 A4177 R4178 L4179 L4183 A4184 W4185 I4189 E4192 R4195 E4206 E4209 R4213 S4214 A4215 C4216 D4217 D4220 L4223 D4224 D4225 K4228 Q4231 K4244 I4251 G4254 D4257 F4260
L4264 T4267 E4270 L4284 K4287 G4290 H4291 P4297 Q4307 W4308 L4311 L4312 Q4316 T4317 P4318 S4319 W4320 L4321 N4325 N4326 R4329 L4344 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 A4375 W4376 T4379 L4380 H4381 W4387 I4391 R4400 T4401 V4402 I4405 K4406 D4407 P4408 L4409 F4410 R4411 F4412 E4416 M4419 L4423 D4430 C4438 K4441 K4442 K4443 Q4444 T4445 N4446 Y4447 L4448 K4457 L4460 P4461 R4462 H4466 Y4467 P4470 M4473 T4474 V4475
I4476 Q4477 A4496 A4497 S4498 G4499 G4500 A4501 K4502 E4503 L4504 K4505 F4515 Y4520 I4521 T4522 Q4526 Y4527 V4528 L4541 E4542 V4543 S4548 Q4549 G4550 A4551 T4552 L4553 D4554 F4558 N4579 L4590 R4591 W4592 N4597 T4598 E4599 K4600 K4601 A4602 P4608 L4611 D4617 L4618 I4619 V4622
I4626 E4630 D4631 P4632 R4633 E4637 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20077	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.167	Depositor
Minimum map value	-0.523	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/23391	0.48	0/31705

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	22907	0	22979	311	0
2	A	81	0	36	3	0
3	A	31	0	12	2	0
4	A	1	0	0	0	0
All	All	23020	0	23027	311	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 7.

All (311) 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:3557:ASP:OD1	1:A:3743:ARG:NH1	2.22	0.73
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.71	0.73
1:A:4225:ASP:O	1:A:4228:LYS:NZ	2.22	0.73
1:A:4267:THR:HG23	1:A:4633:ARG:HD2	1.71	0.71
1:A:2840:ASP:OD1	1:A:2843:ARG:NH2	2.24	0.71
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.72	0.69
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.74	0.69
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.22	0.68
1:A:3851:ASP:HB3	1:A:3854:GLN:HG2	1.73	0.68
1:A:2621:ASN:ND2	1:A:3014:ASN:OD1	2.26	0.67
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.28	0.67
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.75	0.67
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.76	0.66
1:A:1939:GLN:HB3	1:A:1943:ARG:HH12	1.61	0.65
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.32	0.65
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.78	0.65
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.63	0.64
1:A:1647:VAL:HG21	1:A:1666:LEU:HD22	1.78	0.64
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.80	0.64
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.80	0.63
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.80	0.63
1:A:3910:ARG:HE	1:A:4344:LEU:HD11	1.63	0.63
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.78	0.63
1:A:2176:THR:O	1:A:2179:ARG:N	2.33	0.61
1:A:3005:LEU:HD12	1:A:3082:SER:HB2	1.83	0.61
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.82	0.61
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.83	0.61
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.34	0.61
1:A:1985:HIS:HD2	1:A:1997:ILE:HD13	1.66	0.60
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.82	0.59
1:A:2046:ARG:HG3	1:A:2093:LEU:HD22	1.83	0.59
1:A:2075:LEU:HD22	1:A:4522:THR:HG23	1.84	0.59
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.84	0.59
1:A:1708:GLU:HA	1:A:1711:VAL:HG12	1.83	0.59
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.28	0.58
1:A:2457:SER:O	1:A:2461:MET:HG3	2.02	0.58
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.18	0.58
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.83	0.58
1:A:1687:LYS:HG2	1:A:1712:THR:HG23	1.85	0.58
1:A:3488:ARG:NH1	1:A:3746:GLU:OE1	2.36	0.58
1:A:2671:MET:HG2	1:A:2677:GLN:HG3	1.86	0.58
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.86	0.57
1:A:1939:GLN:NE2	1:A:4075:GLU:OE2	2.38	0.57
1:A:1965:GLU:HG2	1:A:2026:SER:HB3	1.85	0.57
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.87	0.57
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	1.86	0.57
1:A:2648:VAL:HG12	1:A:2701:VAL:HG13	1.87	0.57
1:A:4473:MET:HG3	1:A:4477:GLN:HB2	1.85	0.57
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.38	0.56
1:A:1636:ASP:O	1:A:1640:ILE:HD12	2.05	0.56
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.87	0.56
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.85	0.56
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.87	0.56
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.86	0.56
1:A:4192:GLU:HB3	1:A:4321:LEU:HD21	1.88	0.55
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.89	0.55
1:A:2213:ILE:HG22	1:A:2220:LEU:HG	1.88	0.55
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.39	0.55
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.88	0.55
1:A:4409:LEU:HD11	1:A:4558:PHE:HE2	1.72	0.55
1:A:3815:MET:HA	1:A:3818:LEU:HD12	1.89	0.55
1:A:3194:LEU:HD22	1:A:3500:MET:HE3	1.88	0.55
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.07	0.55
1:A:1805:ARG:HD3	1:A:2105:ARG:HH21	1.71	0.54
1:A:3001:ASP:OD1	1:A:3002:SER:N	2.39	0.54
1:A:1985:HIS:CD2	1:A:1997:ILE:HD13	2.42	0.54
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.40	0.54
1:A:2975:ASP:O	1:A:2979:VAL:HG23	2.07	0.54
1:A:2855:LEU:HD21	1:A:2863:ARG:HG3	1.90	0.54
1:A:1943:ARG:NH1	1:A:2273:ARG:HD2	2.23	0.53
1:A:2046:ARG:CG	1:A:2093:LEU:HD22	2.38	0.53
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.89	0.53
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.90	0.53
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.90	0.53
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.08	0.53
1:A:3544:ARG:NH1	1:A:3547:ILE:HG13	2.24	0.53
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.90	0.52
1:A:1582:VAL:HG23	1:A:1591:VAL:HG11	1.90	0.52
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.91	0.52
1:A:1939:GLN:HB3	1:A:1943:ARG:NH1	2.23	0.52
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.45	0.52
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4264:LEU:O	1:A:4267:THR:HB	2.09	0.52
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.89	0.52
1:A:3021:PHE:CG	1:A:3029:LEU:HD22	2.45	0.52
1:A:3123:PRO:HD2	1:A:3126:MET:HE1	1.92	0.52
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.44	0.52
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.90	0.52
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.92	0.52
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.75	0.52
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.28	0.52
1:A:4631:ASP:OD2	1:A:4633:ARG:HB3	2.10	0.52
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.42	0.51
1:A:2925:ILE:HG13	1:A:2933:LEU:HD21	1.90	0.51
1:A:3233:ASN:OD1	1:A:3234:ALA:N	2.43	0.51
1:A:3521:ASP:OD2	1:A:3523:GLN:NE2	2.43	0.51
1:A:4267:THR:HG23	1:A:4633:ARG:CD	2.39	0.51
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.92	0.51
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.92	0.51
1:A:2195:ASP:O	1:A:2198:GLU:HG3	2.11	0.51
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.91	0.51
1:A:3016:GLU:OE1	1:A:3051:TYR:OH	2.27	0.51
1:A:3024:ASP:N	1:A:3024:ASP:OD1	2.43	0.50
1:A:3808:CYS:HB3	1:A:3832:PHE:HZ	1.76	0.50
1:A:2965:ARG:NH2	1:A:3614:PHE:HB3	2.25	0.50
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.44	0.50
1:A:3478:LEU:HD11	1:A:3767:ILE:HG23	1.94	0.50
1:A:1711:VAL:HG23	1:A:1853:VAL:HG21	1.93	0.50
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.44	0.50
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.12	0.49
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.94	0.49
1:A:4500:GLY:H	1:A:4503:GLU:HB3	1.77	0.49
1:A:1664:ILE:HD12	1:A:1666:LEU:HD11	1.95	0.49
1:A:2213:ILE:HA	1:A:2216:ILE:HG22	1.93	0.49
1:A:2046:ARG:HD2	1:A:2070:VAL:HG13	1.94	0.49
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.13	0.49
1:A:3124:ASP:OD1	1:A:3125:TYR:N	2.44	0.49
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.95	0.49
1:A:4065:GLN:HB3	1:A:4092:ARG:HH21	1.78	0.49
1:A:1814:GLU:HB2	1:A:1878:LYS:HE2	1.94	0.49
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.95	0.49
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.47	0.49
1:A:3653:VAL:HG11	1:A:3671:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4402:VAL:O	1:A:4406:LYS:NZ	2.46	0.48
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.48	0.48
1:A:1578:LEU:O	1:A:1582:VAL:HG12	2.13	0.48
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.13	0.48
1:A:3628:ARG:NH2	1:A:3667:GLN:OE1	2.46	0.48
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	1.95	0.48
1:A:3795:GLU:O	1:A:3799:GLN:HG2	2.14	0.48
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.95	0.48
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.13	0.48
1:A:1783:SER:O	1:A:1787:VAL:HG13	2.14	0.48
1:A:2270:PRO:HA	1:A:2273:ARG:HH21	1.77	0.48
1:A:4416:GLU:HA	1:A:4419:MET:HE2	1.94	0.48
1:A:1630:TYR:CE1	1:A:1950:GLN:HG3	2.48	0.48
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.95	0.48
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.32	0.48
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.13	0.48
1:A:3211:THR:O	1:A:3215:VAL:HG13	2.14	0.48
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.14	0.48
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.96	0.48
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.54	0.48
1:A:3725:ASP:HA	1:A:3728:ARG:HG2	1.96	0.47
1:A:4405:ILE:O	1:A:4411:ARG:NE	2.43	0.47
1:A:2221:MET:SD	1:A:2348:LEU:HD11	2.54	0.47
1:A:3738:PHE:CZ	1:A:3783:LYS:HE3	2.48	0.47
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.97	0.47
1:A:2578:GLU:OE1	1:A:2607:SER:OG	2.26	0.47
1:A:4633:ARG:O	1:A:4637:GLU:HG3	2.15	0.47
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.15	0.47
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.95	0.47
1:A:4154:LYS:HD2	1:A:4312:LEU:HB2	1.97	0.47
1:A:2085:HIS:HB3	1:A:2348:LEU:HD12	1.96	0.47
1:A:2163:ASP:OD1	1:A:4526:GLN:NE2	2.31	0.47
1:A:2571:THR:H	1:A:2574:THR:HB	1.80	0.47
1:A:3839:VAL:HG12	1:A:3859:ILE:HG23	1.97	0.47
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.97	0.47
1:A:3060:ARG:HG2	1:A:3060:ARG:HH11	1.80	0.47
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.48	0.47
1:A:2230:LYS:HE2	3:A:4702:ATP:O1B	2.15	0.46
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.48	0.46
1:A:1929:VAL:H	1:A:2332:ARG:HH22	1.63	0.46
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3478:LEU:HD11	1:A:3767:ILE:HG12	1.97	0.46
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.50	0.46
1:A:2642:ARG:NH2	1:A:2704:GLU:OE2	2.48	0.46
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.50	0.46
1:A:2388:ASP:OD1	1:A:2388:ASP:N	2.48	0.46
1:A:2627:THR:OG1	1:A:2629:GLU:OE1	2.22	0.46
1:A:4066:ILE:HD11	1:A:4095:MET:HB2	1.97	0.46
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.97	0.46
1:A:1797:LEU:HD11	1:A:2060:ARG:HH21	1.80	0.46
1:A:4019:SER:O	1:A:4022:GLU:HG2	2.16	0.46
1:A:1632:VAL:HG12	1:A:1656:LYS:HD2	1.97	0.46
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.80	0.46
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	1.98	0.46
1:A:3791:MET:HE2	1:A:3791:MET:HB2	1.74	0.46
1:A:3846:LEU:HD22	1:A:3855:ARG:HG2	1.98	0.46
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.98	0.46
1:A:1543:ARG:HA	1:A:1546:TYR:CZ	2.51	0.45
1:A:3728:ARG:HB3	1:A:3794:VAL:HG11	1.97	0.45
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.96	0.45
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.16	0.45
1:A:2188:GLU:OE1	1:A:2243:ARG:NH2	2.47	0.45
1:A:3644:VAL:HG22	1:A:3664:LEU:HD22	1.99	0.45
1:A:3650:ASN:HD21	1:A:3695:ARG:NH1	2.14	0.45
1:A:3474:ARG:HE	1:A:3767:ILE:HG21	1.82	0.45
1:A:3612:THR:O	1:A:3635:VAL:HA	2.17	0.45
1:A:2517:TYR:CE2	1:A:2521:ILE:HD13	2.52	0.45
1:A:1797:LEU:HD11	1:A:2060:ARG:NH2	2.32	0.45
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.51	0.45
1:A:3855:ARG:O	1:A:3859:ILE:HG13	2.16	0.45
1:A:3929:VAL:O	1:A:3933:GLU:HG3	2.17	0.45
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.99	0.45
1:A:1905:PHE:CE1	1:A:2038:SER:HB2	2.52	0.44
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.35	0.44
1:A:3608:LYS:HB3	1:A:3608:LYS:HE3	1.71	0.44
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.17	0.44
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.99	0.44
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.52	0.44
1:A:1587:LEU:HB3	1:A:1590:ASP:HB2	2.00	0.44
1:A:3194:LEU:HD22	1:A:3500:MET:CE	2.47	0.44
1:A:1985:HIS:CE1	1:A:2010:PRO:HB3	2.52	0.44
1:A:2581:LEU:HD12	1:A:2604:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.58	0.44
1:A:4185:TRP:CD1	1:A:4284:LEU:HD22	2.53	0.44
1:A:4307:GLN:HE22	1:A:4311:LEU:HD11	1.82	0.44
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.52	0.44
1:A:3923:ARG:HG3	1:A:3923:ARG:O	2.17	0.44
1:A:1541:GLN:O	1:A:1545:VAL:HG23	2.18	0.43
1:A:1848:PRO:HA	1:A:1856:GLN:HE21	1.82	0.43
1:A:3214:GLN:O	1:A:3218:LEU:HD23	2.17	0.43
1:A:4174:ASN:OD1	1:A:4231:GLN:NE2	2.49	0.43
1:A:4470:PRO:HD2	1:A:4473:MET:HE3	1.99	0.43
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	2.01	0.43
1:A:3481:SER:HB3	1:A:3774:LYS:HE2	2.00	0.43
1:A:1550:ILE:O	1:A:1554:SER:OG	2.35	0.43
1:A:1911:GLY:HA2	2:A:4701:ADP:H5'1	2.00	0.43
1:A:4376:TRP:HA	1:A:4379:THR:HG22	2.00	0.43
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.01	0.43
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.51	0.43
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	2.00	0.43
1:A:1769:MET:HE2	1:A:1831:ASP:HA	1.99	0.43
1:A:4445:THR:H	1:A:4448:LEU:HB2	1.83	0.43
1:A:2139:GLN:HG3	1:A:2170:TYR:CZ	2.53	0.43
1:A:2414:GLN:NE2	1:A:2418:ASP:OD1	2.51	0.43
1:A:2804:ARG:HG3	1:A:2808:GLU:OE1	2.18	0.43
1:A:2872:LEU:HD22	1:A:2920:LEU:HD12	2.00	0.43
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	2.01	0.43
1:A:3146:SER:HA	1:A:3535:HIS:CE1	2.54	0.43
1:A:3948:ILE:H	1:A:3948:ILE:HD12	1.84	0.43
1:A:1782:LEU:O	1:A:1786:GLU:HG2	2.19	0.43
1:A:2016:ILE:O	1:A:2016:ILE:HG13	2.19	0.43
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	2.01	0.43
1:A:3212:VAL:O	1:A:3215:VAL:HG22	2.19	0.42
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	2.00	0.42
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	2.00	0.42
1:A:1543:ARG:HB3	1:A:1608:LEU:HD12	2.01	0.42
1:A:1959:GLU:HB3	1:A:1962:ARG:CG	2.49	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.42
1:A:4007:MET:O	1:A:4011:THR:HG23	2.20	0.42
1:A:4214:SER:HB2	1:A:4251:ILE:HG23	2.02	0.42
1:A:4467:TYR:HB3	1:A:4515:PHE:HD2	1.84	0.42
1:A:2145:MET:O	1:A:2148:LYS:HG2	2.19	0.42
1:A:3782:ARG:O	1:A:3785:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4048:GLY:HA3	1:A:4206:GLU:OE1	2.20	0.42
1:A:4097:LYS:HA	1:A:4127:THR:OG1	2.19	0.42
1:A:3491:LYS:HA	1:A:3491:LYS:HD3	1.80	0.42
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	2.01	0.42
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	2.02	0.42
1:A:4307:GLN:NE2	1:A:4311:LEU:HD11	2.34	0.42
1:A:4316:GLN:HG3	1:A:4320:TRP:CE3	2.55	0.42
1:A:4626:ILE:HD11	1:A:4632:PRO:HD3	2.02	0.42
1:A:2290:SER:HB2	1:A:2295:LEU:HG	2.02	0.42
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	2.02	0.42
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.55	0.42
1:A:1805:ARG:O	1:A:1809:GLU:HG3	2.20	0.42
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	2.01	0.42
1:A:3221:ASP:O	1:A:3225:LYS:HG2	2.20	0.42
1:A:3617:ASP:N	1:A:3617:ASP:OD1	2.52	0.42
1:A:1613:LYS:O	1:A:1617:GLU:HG2	2.20	0.41
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	2.02	0.41
1:A:2059:PHE:CZ	1:A:2104:LYS:HD3	2.55	0.41
1:A:2232:MET:HE2	1:A:2232:MET:HA	2.01	0.41
1:A:1847:ASP:O	1:A:1856:GLN:HG3	2.21	0.41
1:A:1888:CYS:HA	1:A:2039:LEU:CD2	2.50	0.41
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	2.02	0.41
1:A:2536:ASP:OD1	1:A:2572:LEU:HD21	2.20	0.41
1:A:2962:LYS:HG3	1:A:3665:GLY:HA2	2.02	0.41
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.53	0.41
1:A:3544:ARG:HH12	1:A:3547:ILE:HG13	1.85	0.41
1:A:4057:ASP:O	1:A:4061:GLU:HG2	2.21	0.41
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.20	0.41
1:A:3454:LEU:O	1:A:3457:GLU:HG2	2.21	0.41
1:A:3691:ASP:O	1:A:3695:ARG:HG3	2.21	0.41
1:A:2306:ASP:OD2	1:A:2676:THR:OG1	2.29	0.41
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	2.02	0.41
1:A:4209:GLU:OE2	1:A:4213:ARG:NE	2.54	0.41
1:A:1560:LEU:O	1:A:1561:LEU:HD23	2.21	0.41
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	2.03	0.41
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.84	0.41
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.01	0.41
1:A:2144:THR:HG22	1:A:2145:MET:HE2	2.02	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.56	0.41
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.56	0.41
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3740:LEU:O	1:A:3744:GLN:HG3	2.21	0.41
1:A:3759:ARG:HH21	1:A:3761:LEU:HB2	1.85	0.41
1:A:4260:PHE:CZ	1:A:4608:PRO:HB3	2.56	0.41
1:A:2507:ARG:HE	1:A:2507:ARG:HB2	1.70	0.41
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.69	0.41
1:A:2107:ARG:NH1	1:A:2135:GLU:OE2	2.54	0.40
1:A:3159:ALA:O	1:A:3163:LYS:HG2	2.21	0.40
1:A:4168:ARG:NH2	1:A:4217:ASP:OD2	2.48	0.40
1:A:1679:ARG:H	1:A:1679:ARG:HD2	1.86	0.40
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	2.04	0.40
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.86	0.40
1:A:1914:GLU:HG2	2:A:4701:ADP:O1A	2.21	0.40
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.56	0.40
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	2.04	0.40
1:A:1848:PRO:HA	1:A:1856:GLN:NE2	2.36	0.40
1:A:3075:LEU:HD12	1:A:3075:LEU:HA	1.95	0.40
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.57	0.40
1:A:1787:VAL:O	1:A:1791:VAL:HG23	2.22	0.40
1:A:2046:ARG:HG2	1:A:2070:VAL:HG22	2.03	0.40
1:A:2717:ASP:O	1:A:4446:ASN:ND2	2.53	0.40
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.51	0.40
1:A:4244:LYS:NZ	1:A:4270:GLU:OE1	2.53	0.40
1:A:4387:TRP:O	1:A:4391:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2849/4646 (61%)	2808 (99%)	41 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	2530/4125 (61%)	2529 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3607	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1856	GLN
1	A	1985	HIS
1	A	2621	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	ATP	A	4702	4	28,33,33	0.74	0	34,52,52	0.79	1 (2%)
2	ADP	A	4703	-	24,29,29	0.72	0	29,45,45	0.73	1 (3%)
2	ADP	A	4701	-	24,29,29	0.74	0	29,45,45	0.75	1 (3%)
2	ADP	A	4704	-	24,29,29	0.75	0	29,45,45	0.74	1 (3%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4703	ADP	C5-C6-N6	2.30	123.82	120.31
2	A	4704	ADP	C5-C6-N6	2.29	123.81	120.31
2	A	4701	ADP	C5-C6-N6	2.28	123.78	120.31
3	A	4702	ATP	C5-C6-N6	2.25	123.73	120.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	PA-O3A-PB-O3B
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	O4'-C4'-C5'-O5'

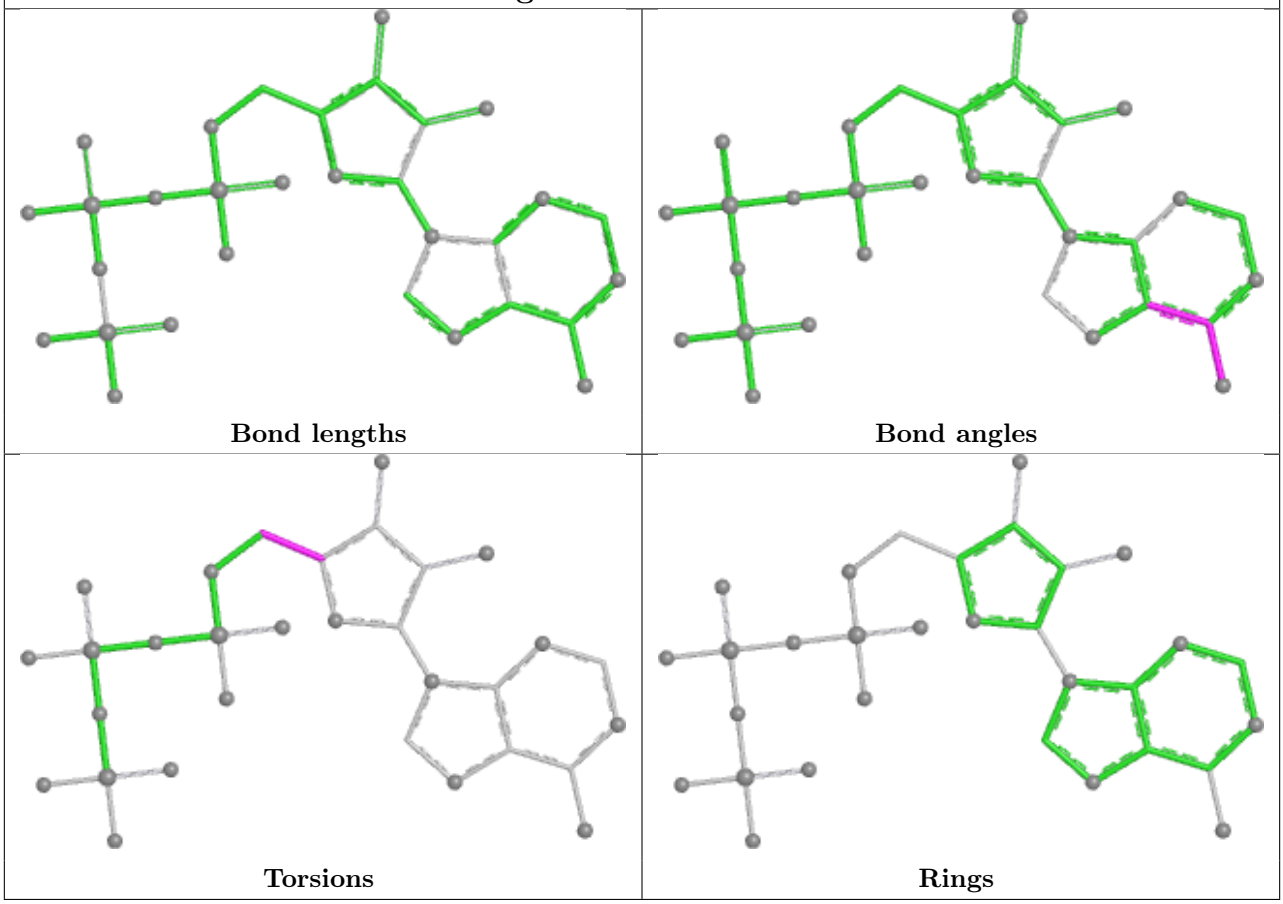
There are no ring outliers.

2 monomers are involved in 5 short contacts:

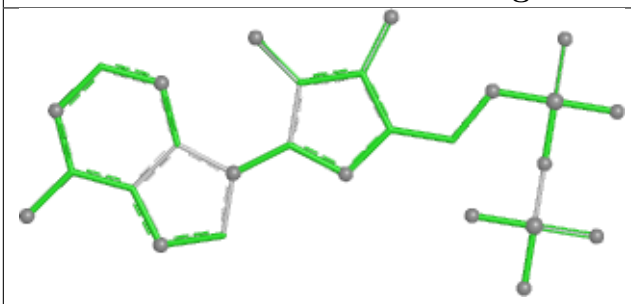
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	2	0
2	A	4701	ADP	3	0

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.

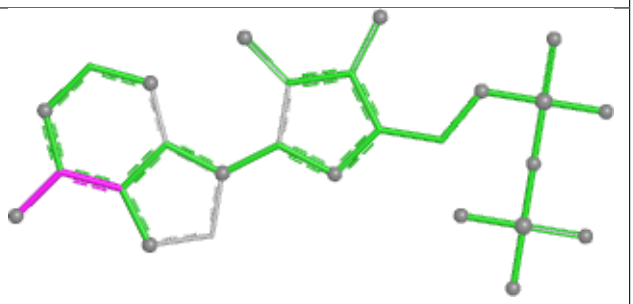
Ligand ATP A 4702



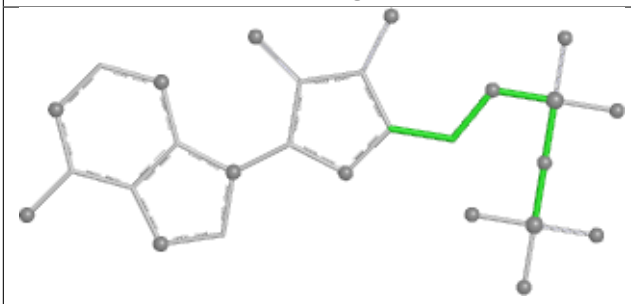
Ligand ADP A 4703



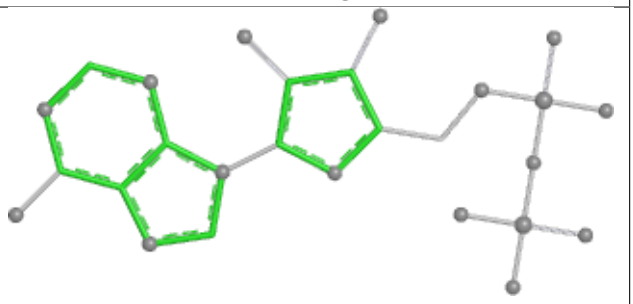
Bond lengths



Bond angles

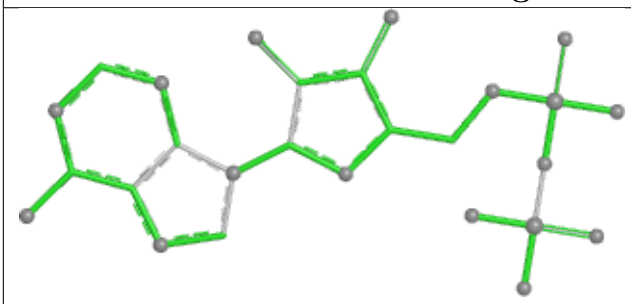


Torsions

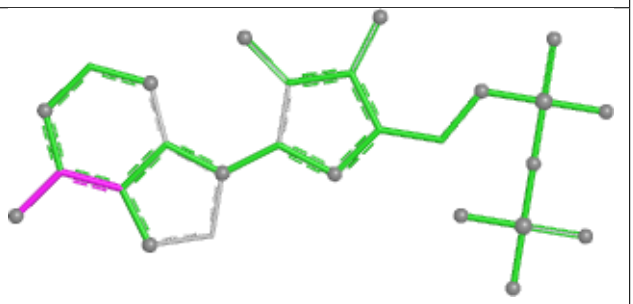


Rings

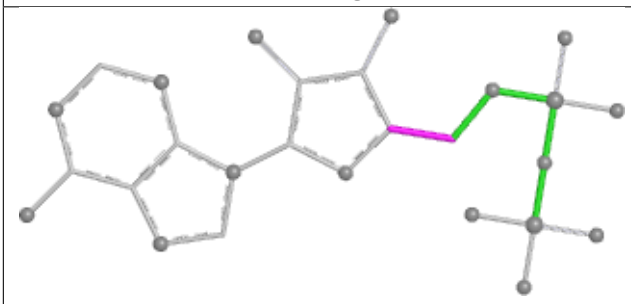
Ligand ADP A 4701



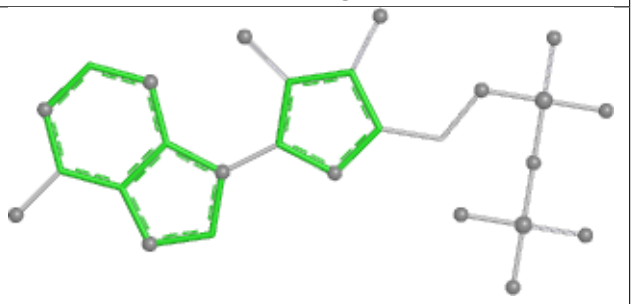
Bond lengths



Bond angles

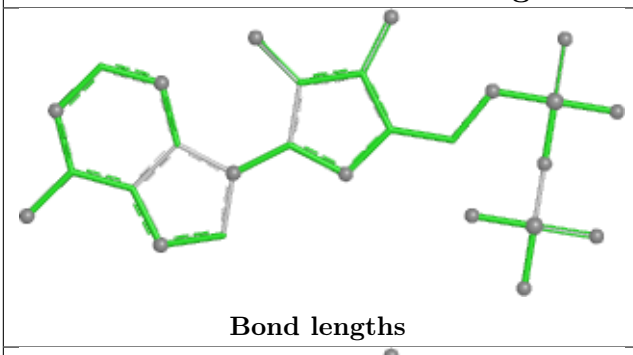


Torsions

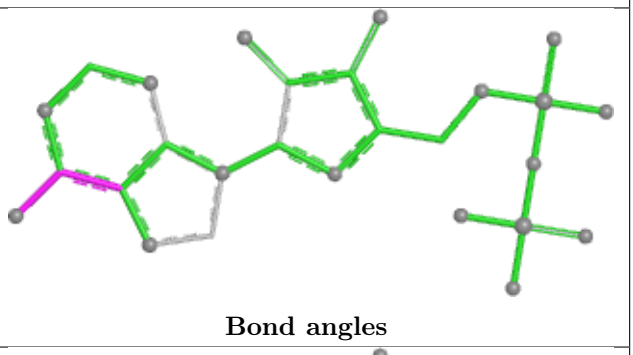


Rings

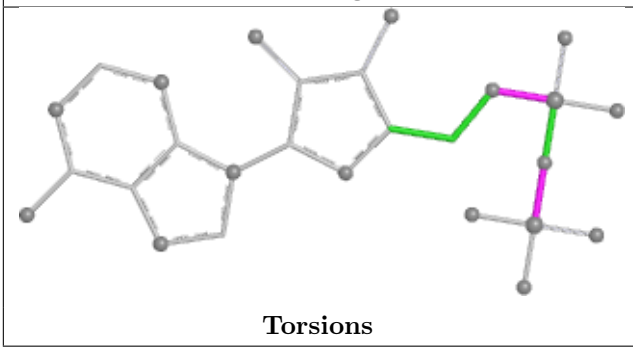
Ligand ADP A 4704



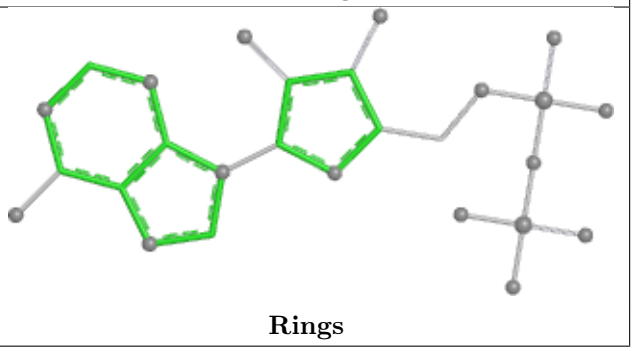
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

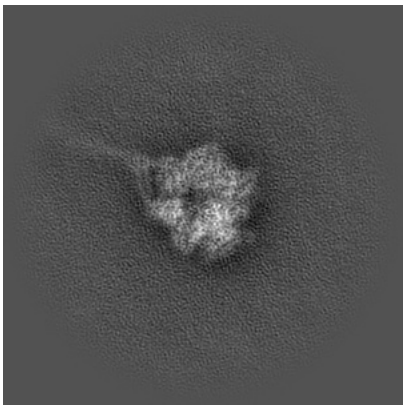
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46858. These allow visual inspection of the internal detail of the map and identification of artifacts.

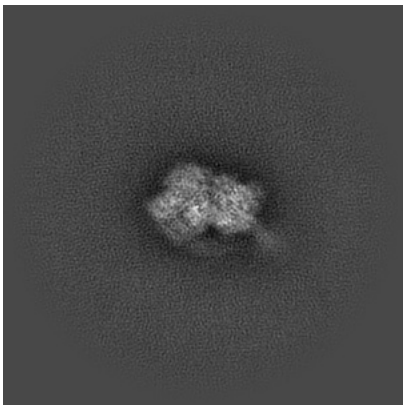
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

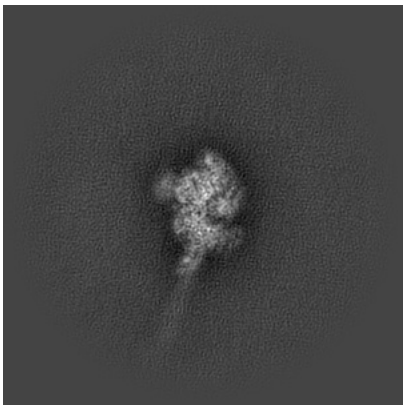
6.1.1 Primary map



X

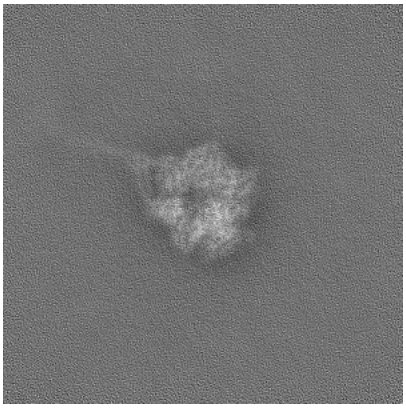


Y

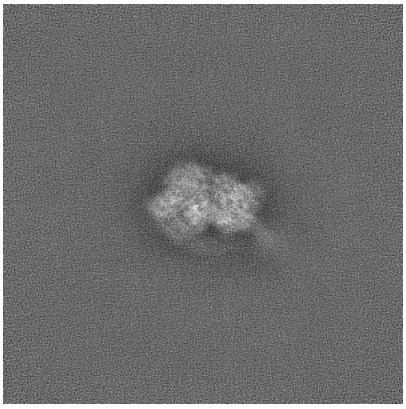


Z

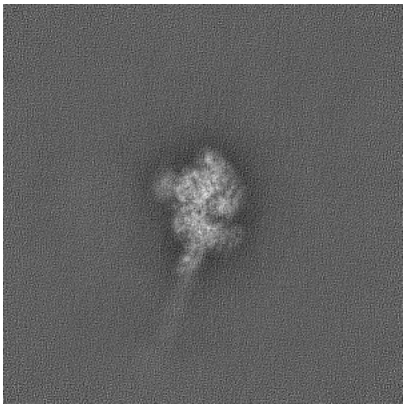
6.1.2 Raw map



X



Y

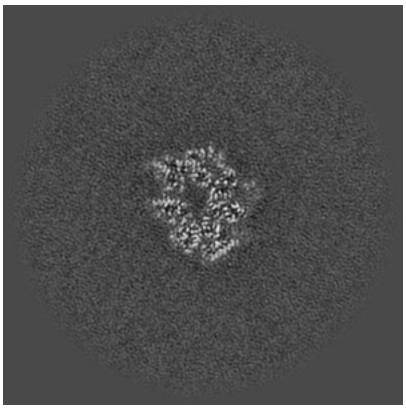


Z

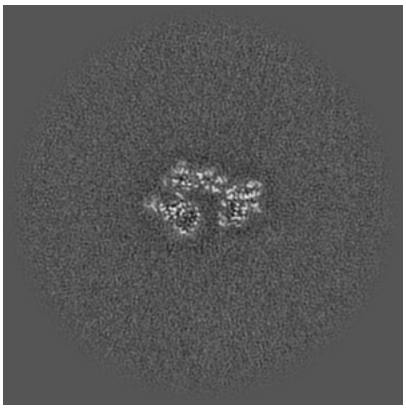
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

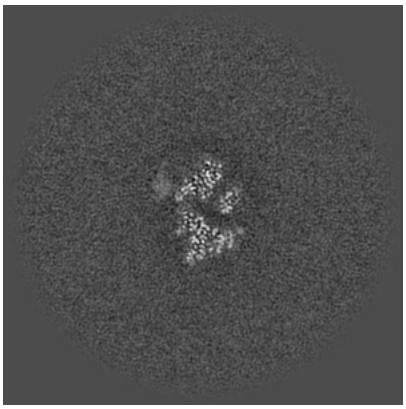
6.2.1 Primary map



X Index: 192

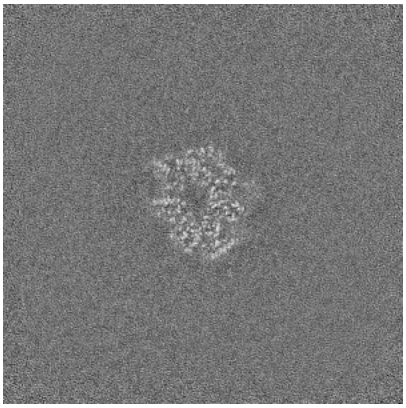


Y Index: 192

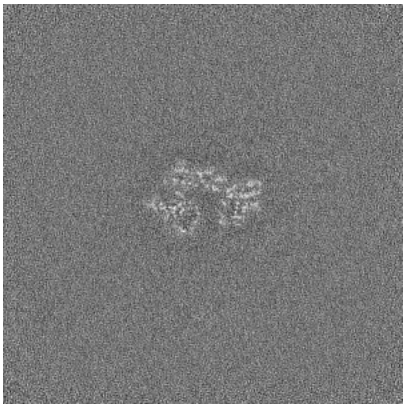


Z Index: 192

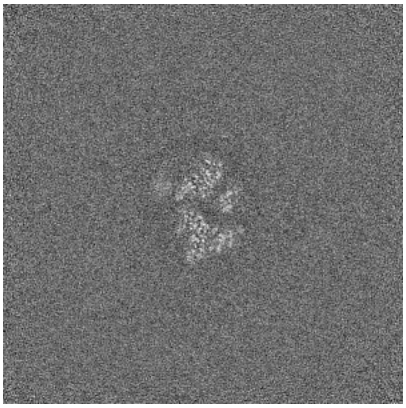
6.2.2 Raw map



X Index: 192



Y Index: 192

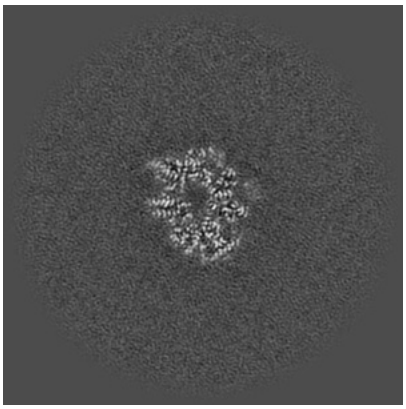


Z Index: 192

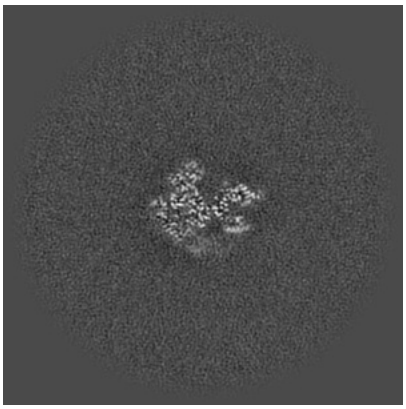
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

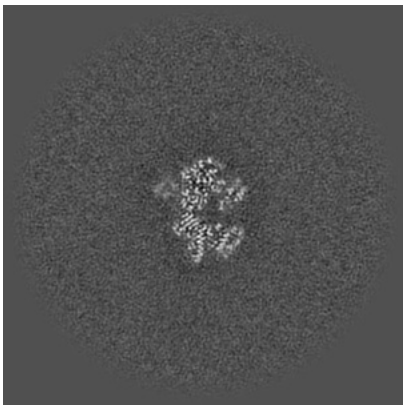
6.3.1 Primary map



X Index: 191

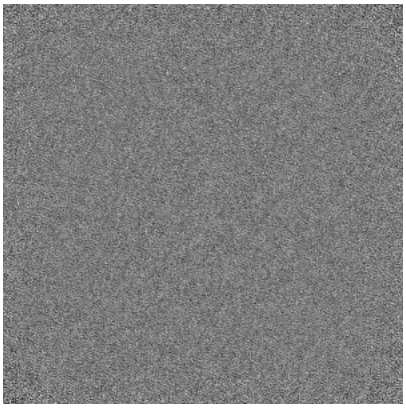


Y Index: 206

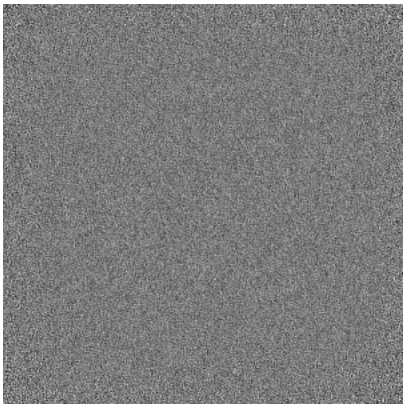


Z Index: 184

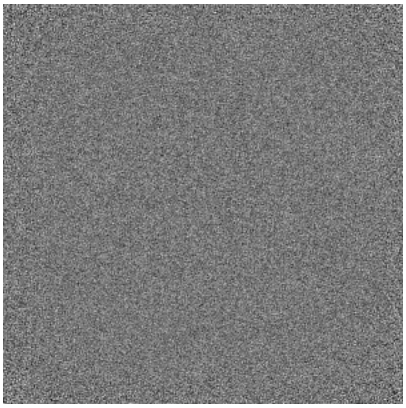
6.3.2 Raw map



X Index: 0



Y Index: 0

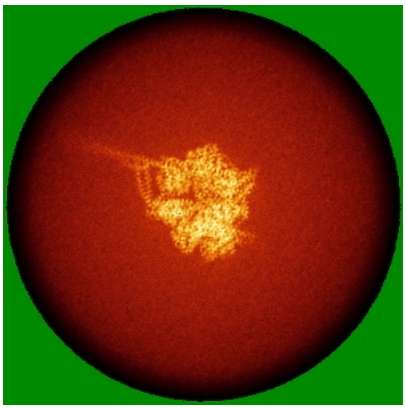


Z Index: 0

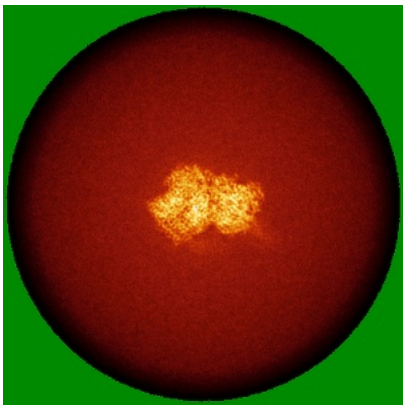
The images above show the largest variance slices of the map in three orthogonal directions.

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

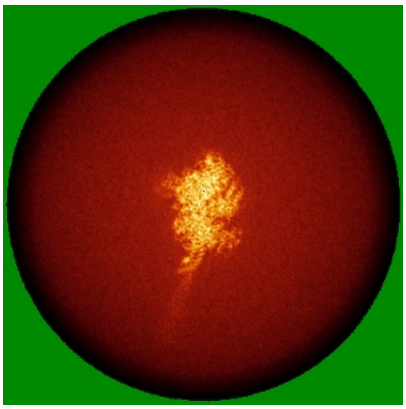
6.4.1 Primary map



X

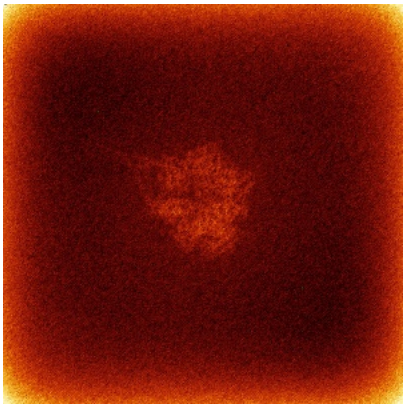


Y

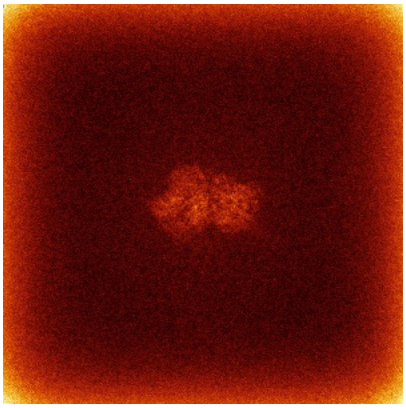


Z

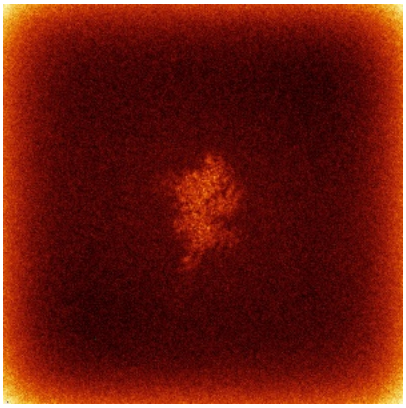
6.4.2 Raw map



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.

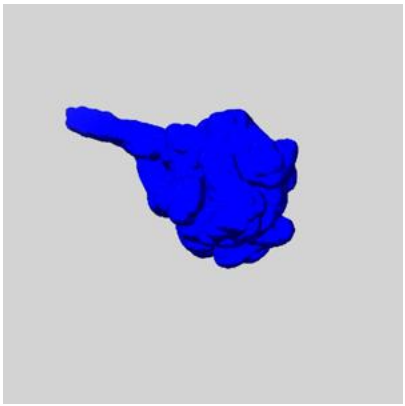
6.6 Mask visualisation (i)

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

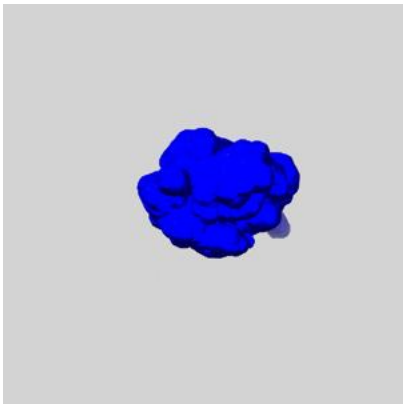
A mask typically either:

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

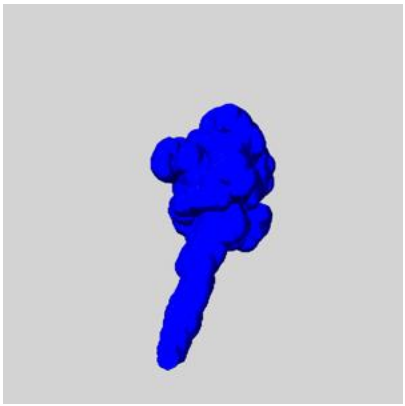
6.6.1 emd_46858_msk_1.map (i)



X



Y

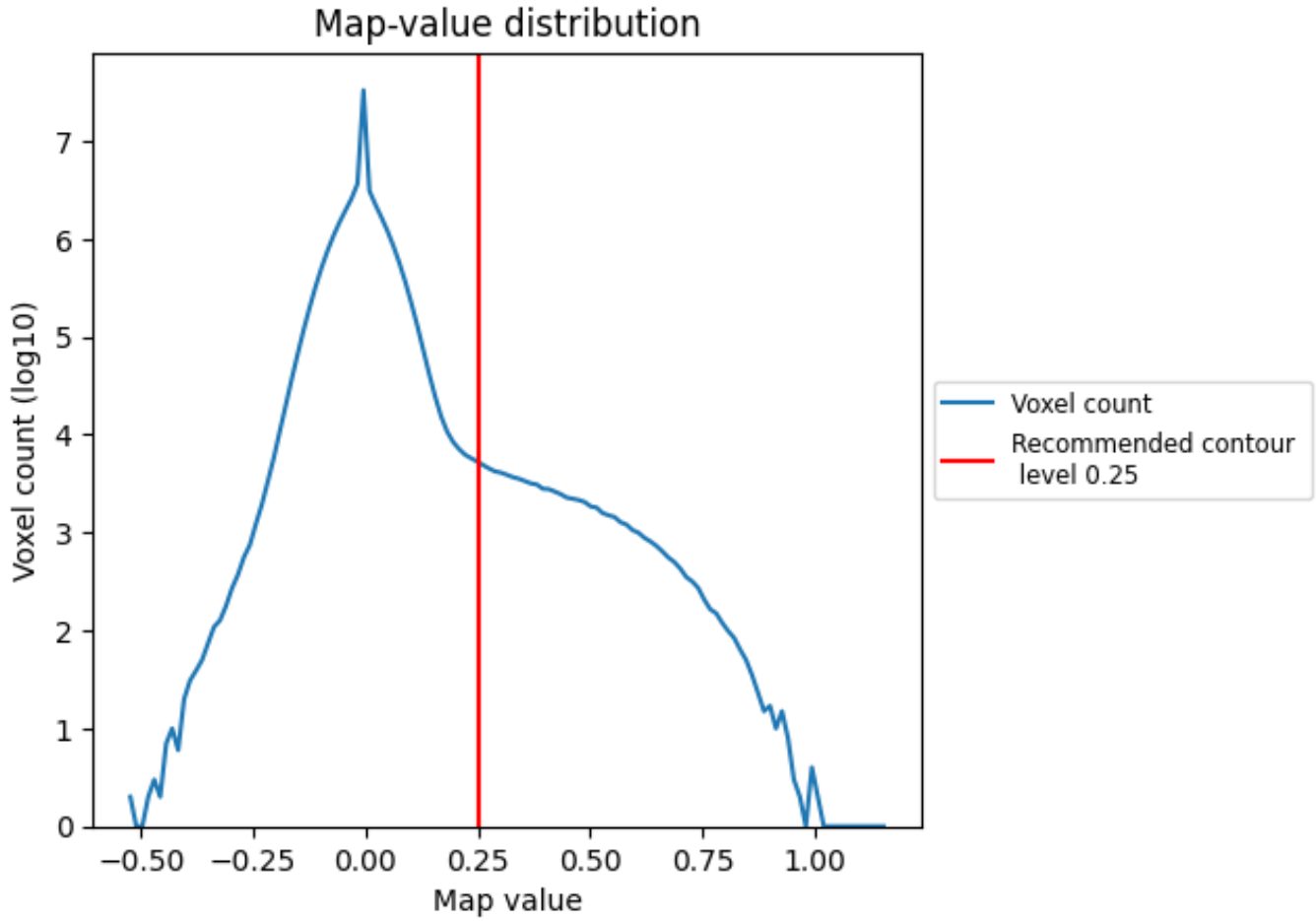


Z

7 Map analysis

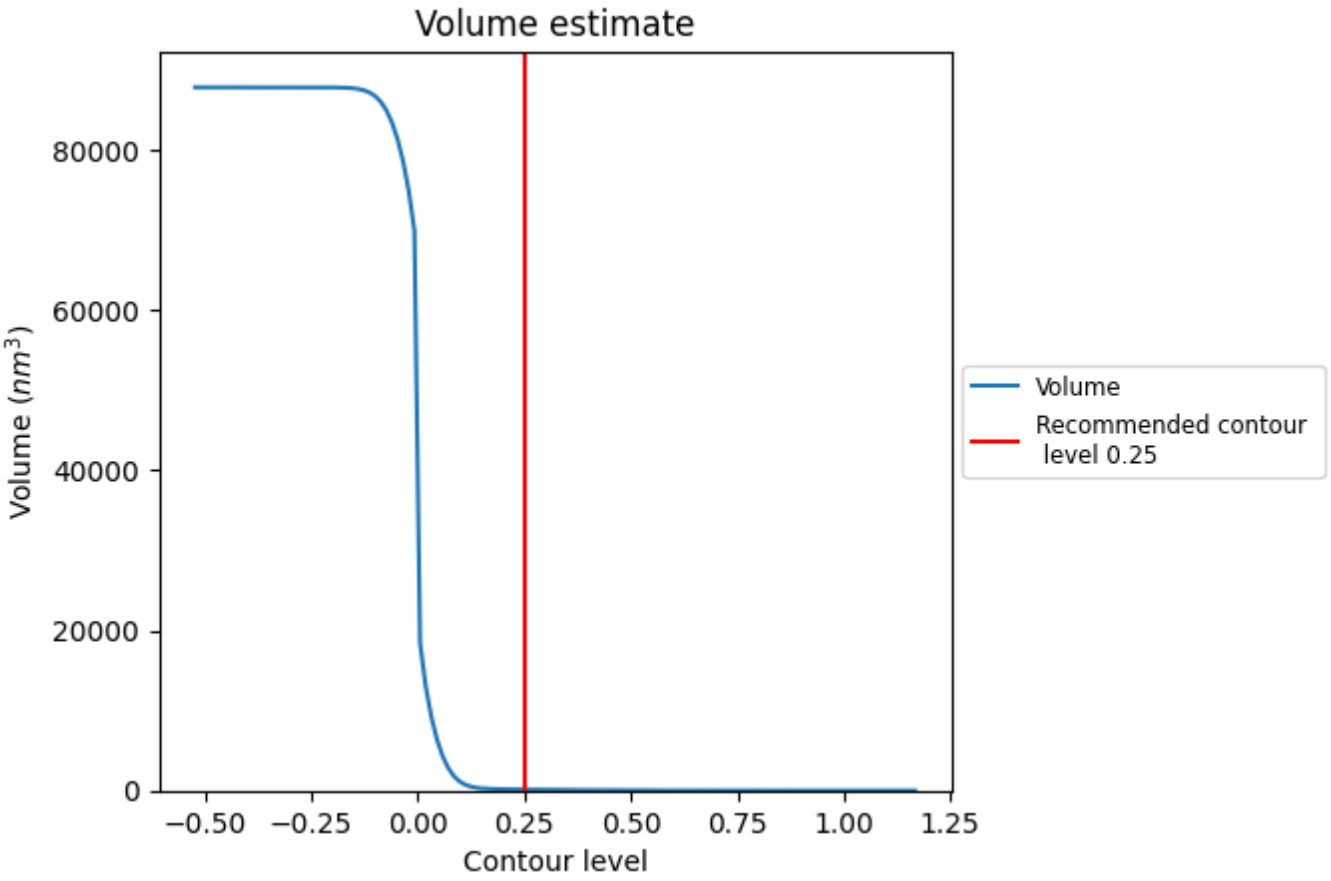
This section contains the results of statistical analysis of the map.

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.

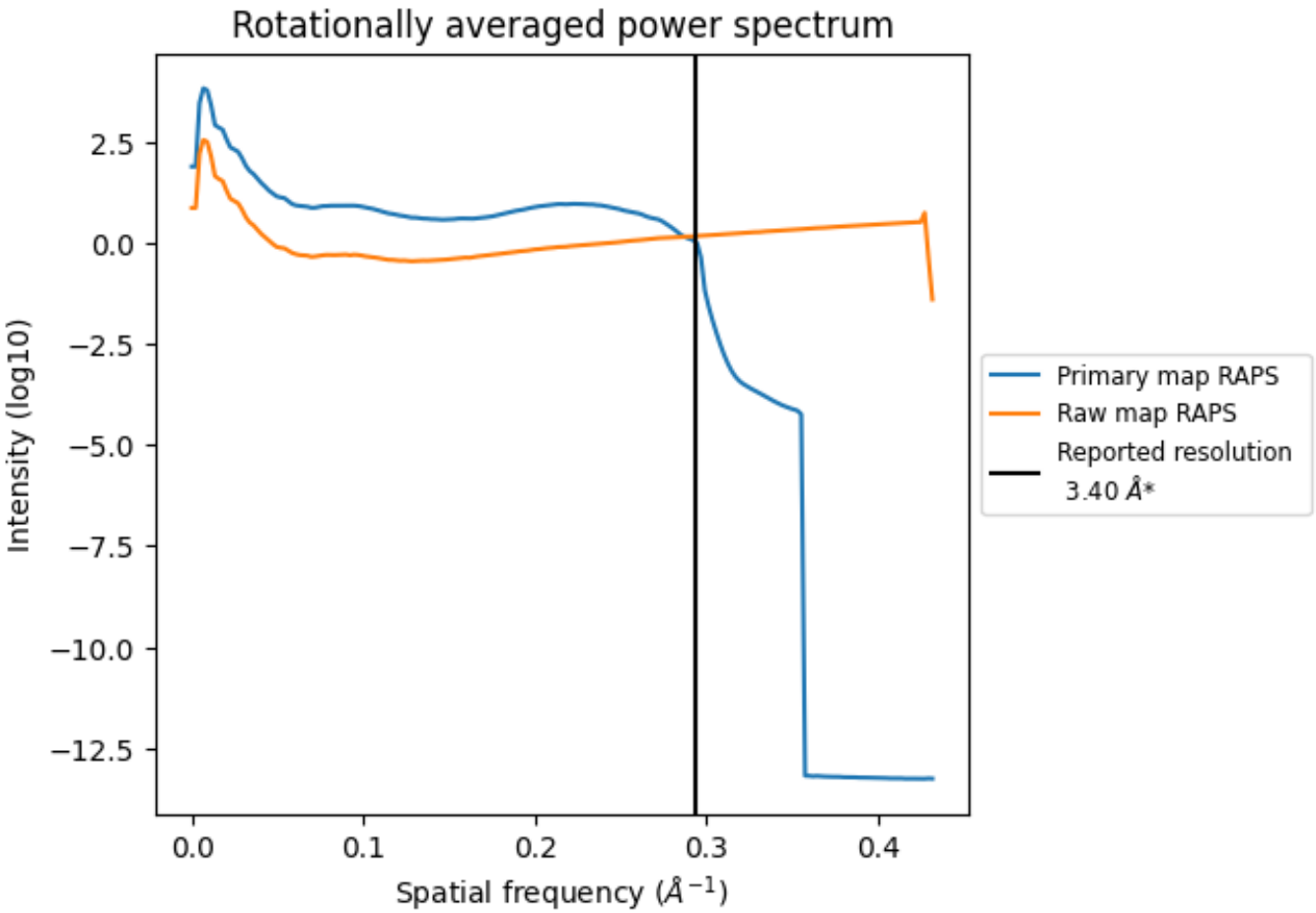
7.2 Volume estimate



The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 kDa.

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

7.3 Rotationally averaged power spectrum (i)

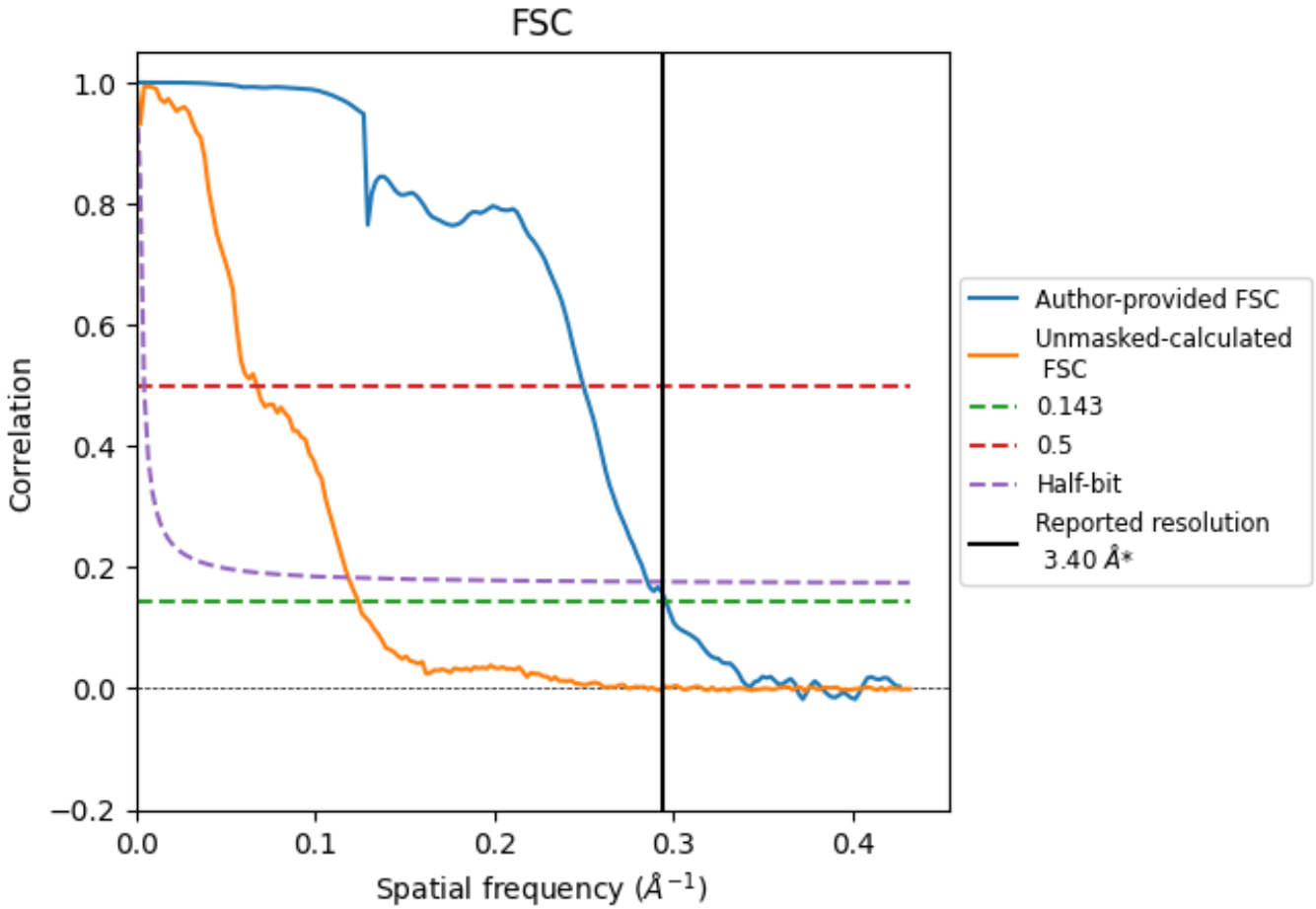


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

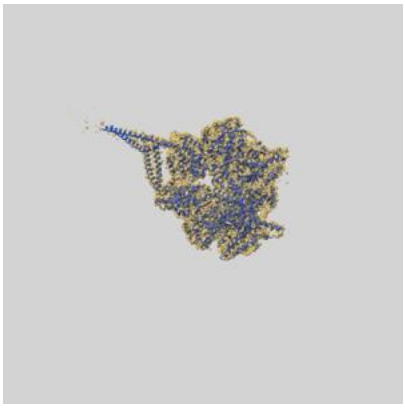
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	4.00	3.50
Unmasked-calculated*	8.06	14.84	8.43

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

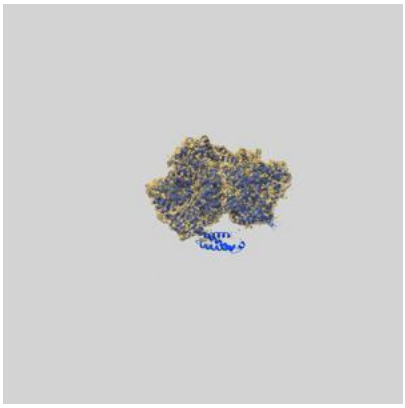
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46858 and PDB model 9DH7. Per-residue inclusion information can be found in section 3 on page 5.

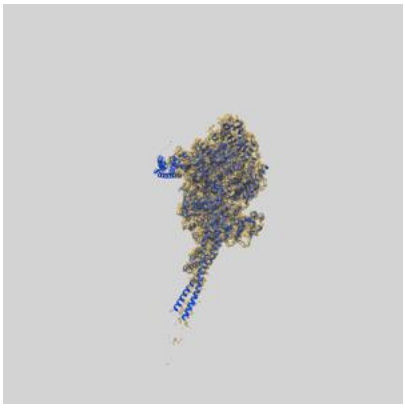
9.1 Map-model overlay



X



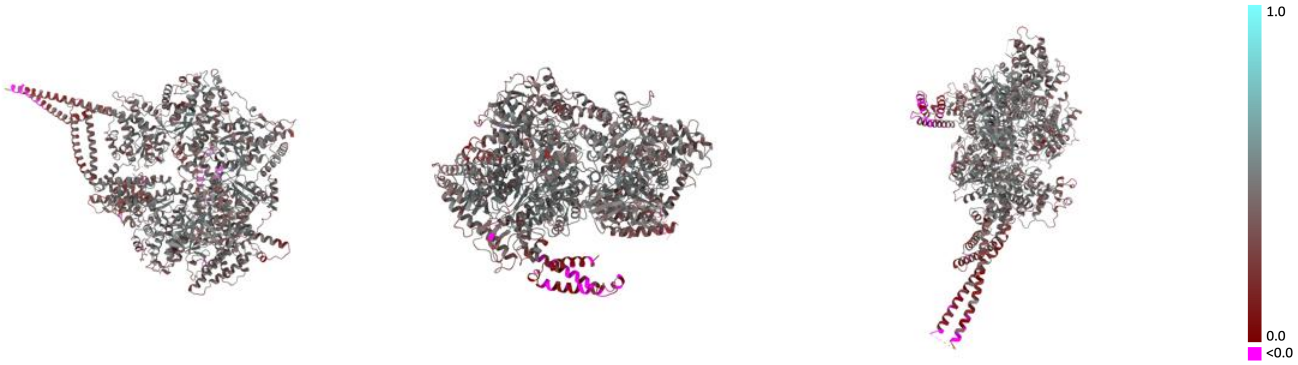
Y



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.

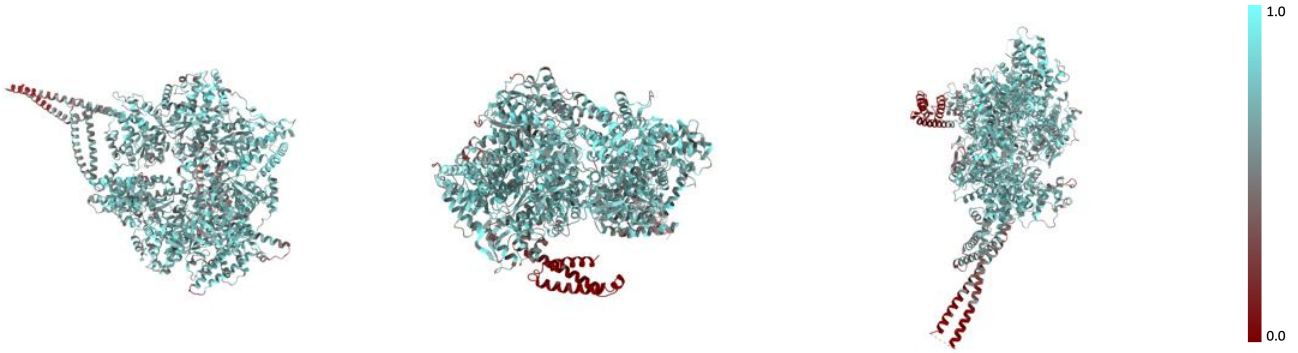
9.2 Q-score mapped to coordinate model (i)



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.

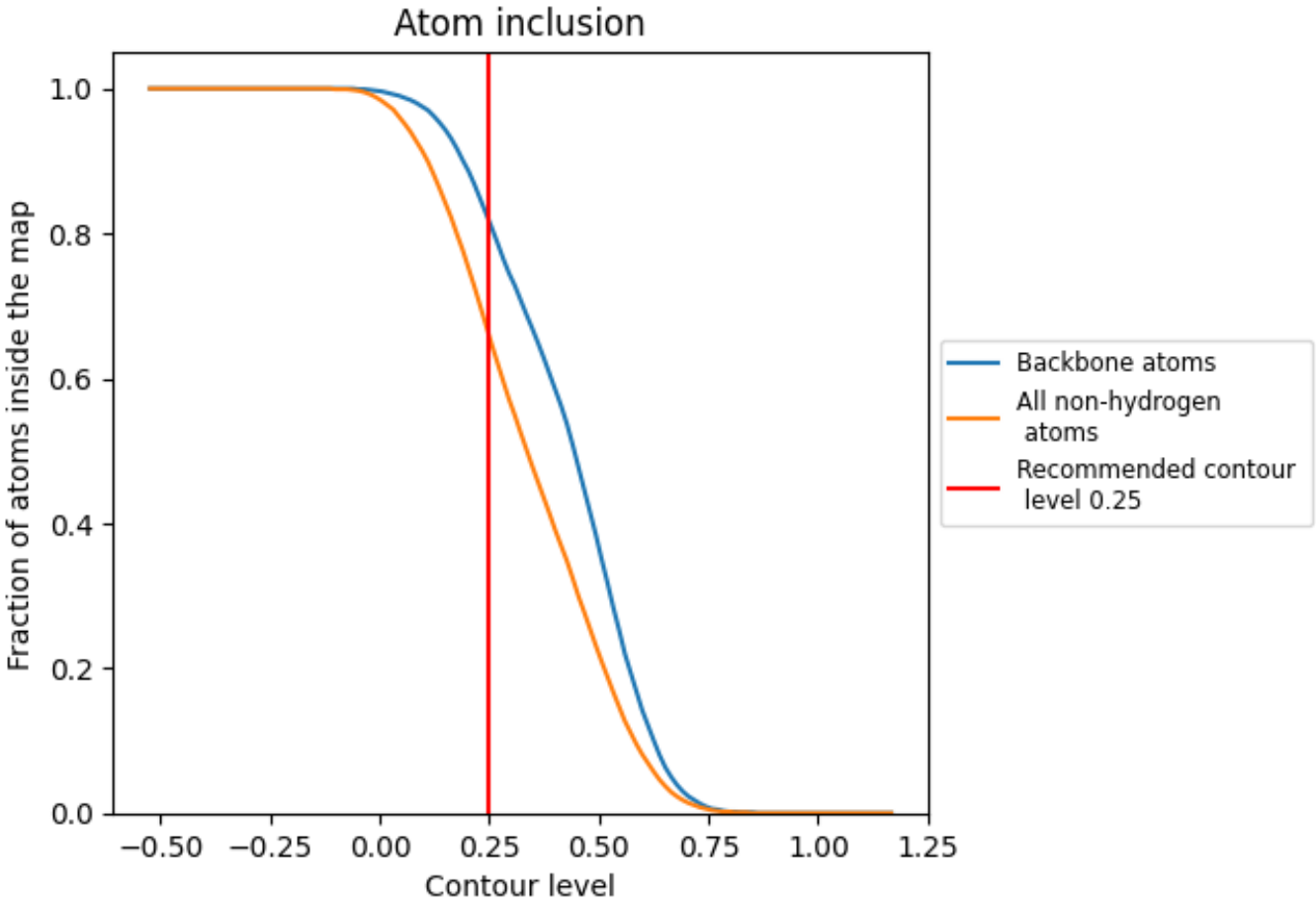
9.3 Atom inclusion mapped to coordinate model (i)



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, 82% of all backbone atoms, 66% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.4120
A	0.6580	0.4120