Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 04:12 PM EDT

PDB ID	:	9DH6 / pdb_00009dh6
EMDB ID	:	EMD-46857
Title	:	State-2 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:

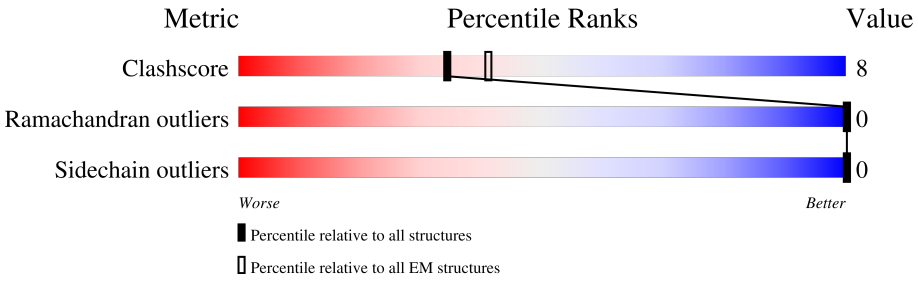
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 3.40 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	26% 51% 13% 37%

2 Entry composition

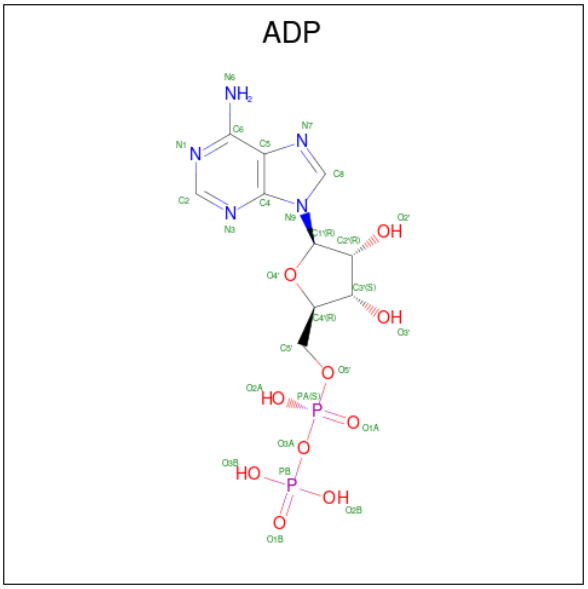
There are 4 unique types of molecules in this entry. The entry contains 23689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

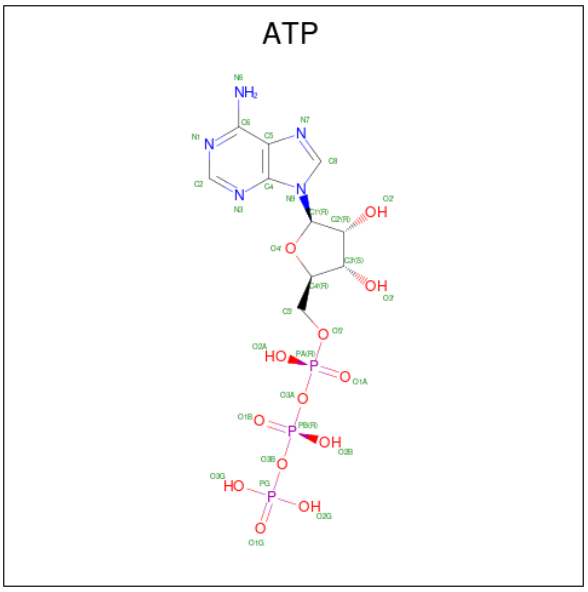
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2935	23575	15017	4067	4374	117	0	0

- 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).

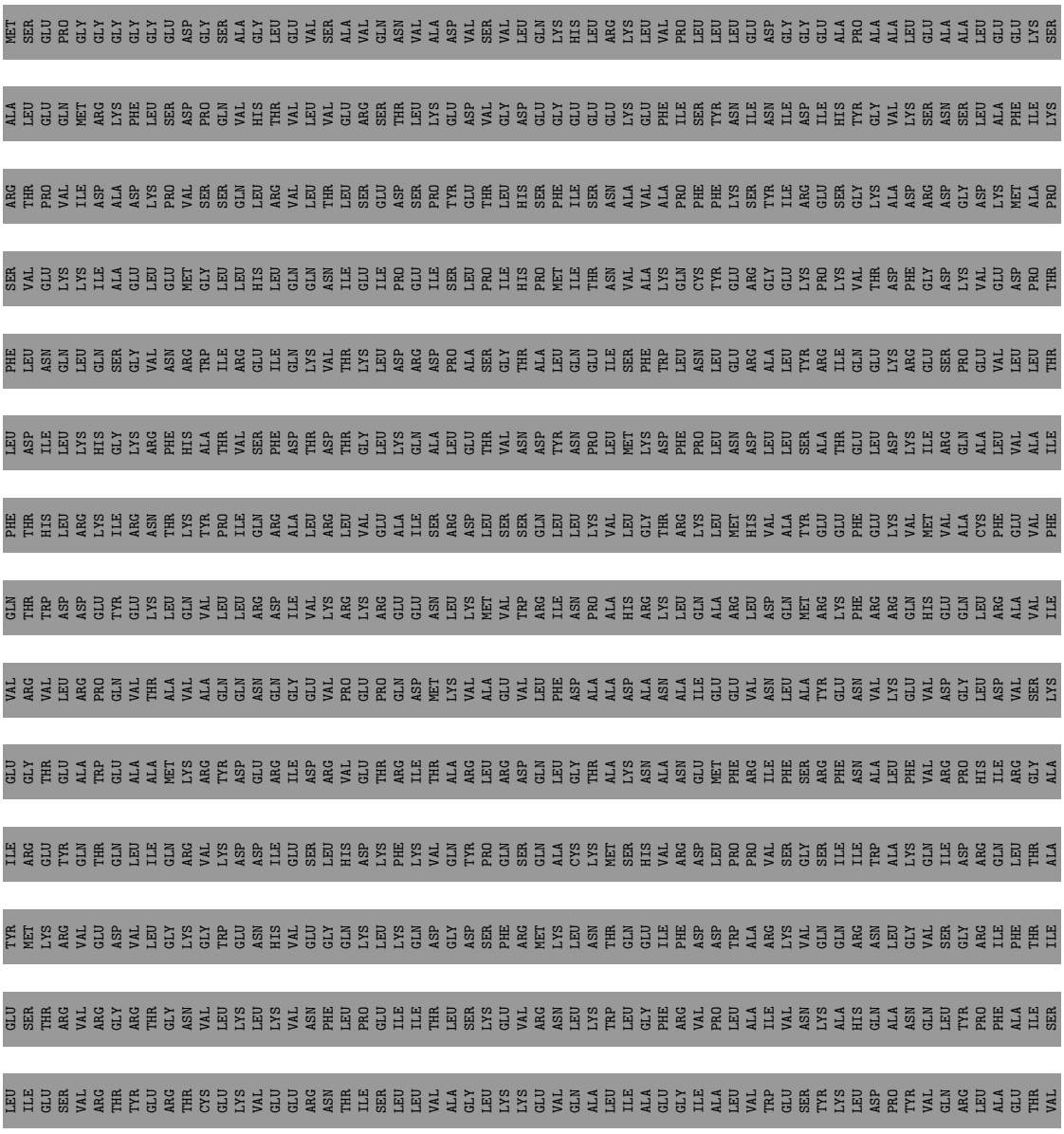
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	

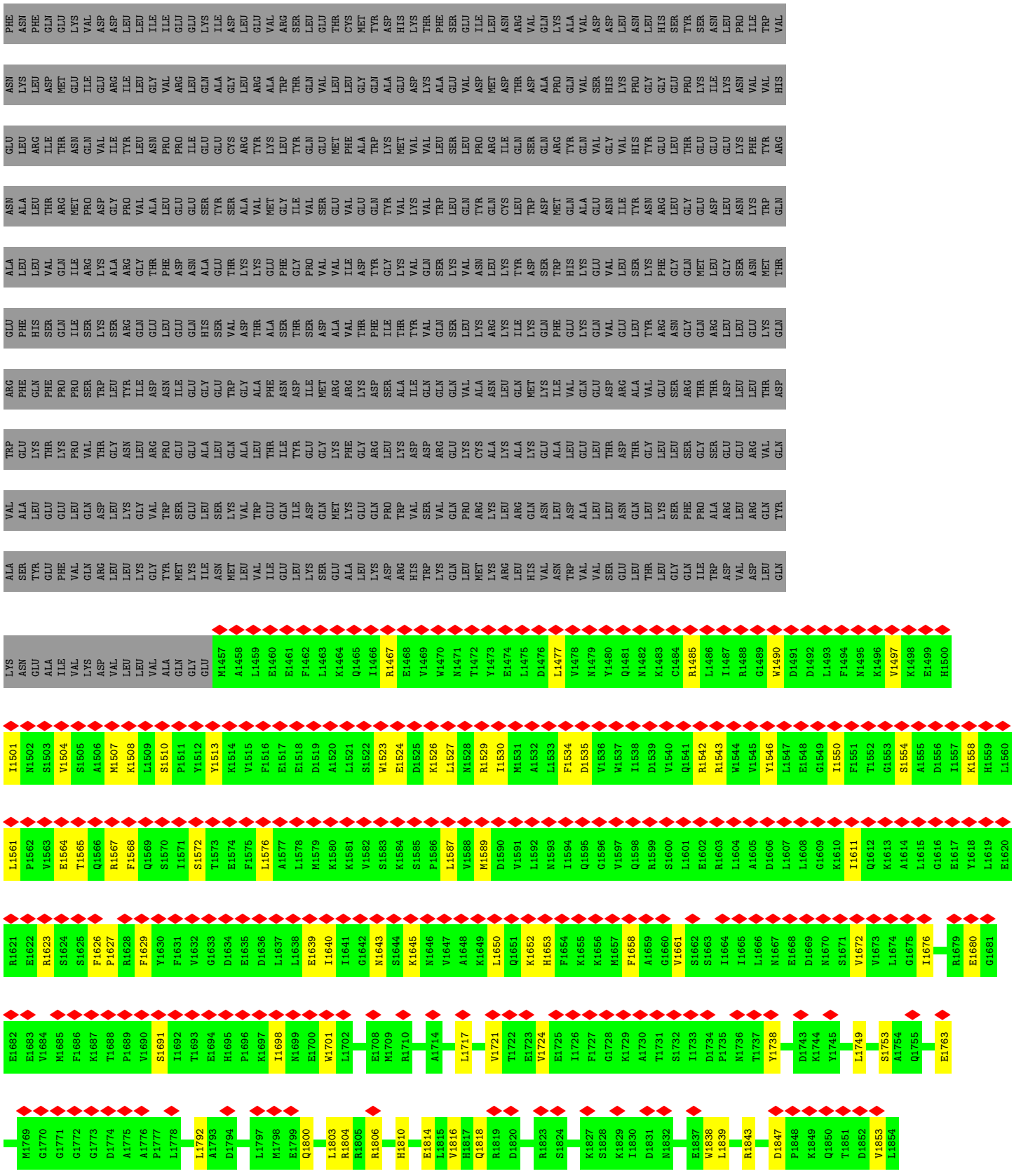
3 Residue-property plots (i)

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

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain A:




PHE ASN PHE GLN GLU LYS VAL ASP ASP LEU LEU ILE ILE GLU GLU LYS ILE ASP LEU GLU VAL ARG SER LEU GLU THR CYS MET TYR ASP HIS LYS THR PHE SER GLU ILE LEU ASN ARG VAL GLN LYS ALA VAL ASP ASP LEU ASN LEU LEU HIS SER TYR SER ASN LEU PRO ILE VAL TRP VAL
ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU 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 GLU VAL ASP MET ASP THR ASP ALA PRO GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS
GLU LEU ARG ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU GLU SER LEU PRO ARG GLN ILE GLN SER GLN ARG TYR GLN VAL GLY VAL HIS TYR ASN ARG 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 ASN ILE GLN CYS LEU TRP ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS TRP GLN
ALA LEU LEU VAL GLN ILE ARG LYS ALA ARG GLY THR PHE ASP ASN ALA GLU THR LYS LYS GLU PHE GLY PRO VAL VAL ILE ASP TYR GLY LYS VAL GLN SER LYS VAL ASN LEU GLN 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 VAL PRO VAL ALA ILE THR THR TYR ARG ASN GLY GLN LEU LYS ARG LYS ILE LYS GLN PHE GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN GLU LEU LEU GLU LYS GLN
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ILE MET ARG ARG LYS ASP SER ALA ILE ASP ALA ARG ALA VAL GLN GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP ASP LEU ASP THR
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 GLU ARG VAL GLN
VAL ALA LEU 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 LEU ARG GLN PRO TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN LEU ASP ALA LEU LEU LEU ASN GLN LEU 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 LEU VAL ALA GLN GLY GLU M1457 A1458 L1459 E1460 E1461 F1462 L1463 K1464 Q1465 I1466 R1467 E1468 V1469 W1470 N1471 T1472 Y1473 E1474 L1475 D1476 L1477 V1478 N1479 Y1480 Q1481 N1482 K1483 C1484 R1485 I1486 I1487 R1488 G1489 W1490 D1491 D1492 L1493 F1494 N1495 K1496 V1497 K1498 E1499 H1500
I1501 N1502 S1503 V1504 S1505 A1506 M1507 K1508 L1509 S1510 P1511 Y1512 Y1513 K1514 V1515 F1516 E1517 E1518 D1519 A1520 L1521 S1522 W1523 E1524 D1525 K1526 L1527 N1528 R1529 I1530 M1531 A1532 L1533 F1534 D1535 V1536 W1537 I1538 D1539 V1540 Q1541 R1542 R1543 W1544 Y1545 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 R1623 S1624 S1625 F1626 P1627 R1628 F1629 Y1630 F1631 V1632 G1633 D1634 E1635 D1636 L1637 L1638 E1639 I1640 I1641 G1642 N1643 S1644 K1645 N1646 V1647 A1648 K1649 L1650 Q1651 K1652 H1653 F1654 K1655 K1656 M1657 F1658 A1659 G1660 V1661 S1662 S1663 I1664 I1665 L1666 N1667 E1668 D1669 N1670 S1671 V1672 V1673 L1674 G1675 I1676 R1679 E1680 G1681
E1682 E1683 V1684 M1685 F1686 K1687 T1688 P1689 V1690 S1691 I1692 T1693 E1694 H1695 P1696 K1697 I1698 N1699 E1700 W1701 L1702 E1708 M1709 R1710 A1714 L1717 V1721 T1722 E1723 V1724 E1725 I1726 F1727 G1728 K1729 A1730 T1731 S1732 I1733 D1734 P1735 N1736 T1737 Y1738 D1743 K1744 Y1745 L1749 S1753 A1754 Q1755 E1763
M1769 G1770 G1771 G1772 G1773 D1774 A1775 A1776 P1777 L1778 L1792 A1793 D1794 L1797 M1798 E1799 Q1800 L1803 R1804 R1805 R1806 H1810 E1814 L1815 V1816 H1817 Q1818 R1819 D1820 R1823 S1824 K1827 S1828 K1829 I1830 D1831 N1832 E1837 W1838 L1839 R1843 D1847 P1848 K1849 Q1850 T1851 D1852 V1853 L1854


Q1855 Q1856 K1865 E1871 Q1876 D1877 K1878 L1879 V1880 Q1881 D1886 R1887 M1892 R1899 S1903 P1904 A1908 K1912 T1913 E1914 H1921 R1925 F1926 F1930 D1933 E1934 T1935 F1936 D1937 F1938 Q1939 A1940 M1941 G1942 R1943 Q1950 F1957 D1958 E1959 F1960 E1964 E1965 R1966
S1969 A1970 V1971 S1972 E1980 A1981 L1982 R1983 E1984 H1985 S1986 N1987 P1988 N1989 Y1990 D1991 K1992 T1993 S1994 A1995 P1996 I1997 T1998 C1999 E2000 L2001 L2002 N2003 K2004 Q2005 V2006 P2010 D2011 I2016 T2017 M2018 G2021 Y2022 A2023 G2024 R2025 S2026 N2027 L2028 P2029 D2030 N2031 L2032 K2033 K2034 T2042 K2043 P2044 D2045 R2046
Q2047 V2052 M2053 R2060 E2063 A2066 N2067 K2068 I2069 V2070 P2071 L2075 C2076 D2077 E2078 Q2079 L2080 S2081 S2082 Q2083 D2087 R2091 A2092 L2093 K2094 N2102 V2103 K2104 R2105 E2106 R2107 I2108 Q2109 K2110 I2111 K2112 R2113 E2114 K2115 E2116 E2117 R2118 G2119 E2120 A2121 V2122 D2123 E2124 G2125 E2126 I2127 A2128
E2129 N2130 L2131 E2135 I2138 M2145 K2148 L2149 V2150 A2151 E2152 L2156 L2157 F2158 S2159 L2160 L2161 S2162 D2163 V2164 F2165 P2166 G2167 V2168 Q2169 Y2170 H2171 R2172 G2173 E2174 M2175 T2176 A2177 L2178 R2179 E2180 E2181 Q2187 D2195 G2196 E2197 E2198 E2205 Q2212 M2221 G2224 S2228
S2231 W2234 E2242 R2243 L2244 E2245 E2248 D2255 P2256 K2257 A2258 H2263 L2268 D2269 P2270 N2271 T2272 R2273 E2274 W2275 T2276 D2277 R2285 K2286 D2289 S2290 V2291 R2292 G2293 E2294 L2295 Q2296 K2297 R2298 D2304 G2305 D2306 V2307 D2308 P2309 E2310 W2311 V2312 E2313 N2316 D2320 D2321 N2322 K2323
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GLU GLY GLU GLU ALA ALA S2410 P2411 M2412 L2413 Q2416 R2417 D2418 I2422 M2423 Q2424 N2430 G2431 L2432 V2433 E2438 H2439 A2440 F2441 Q2442 L2443 E2444 H2445 I2446 M2447 D2448 L2449 T2450 R2451 L2452 R2453 S2457 M2461 L2462 H2463 Q2464 A2465 C2466 R2467 Q2471 N2475 H2476 P2477 D2478 F2479 P2480 M2481
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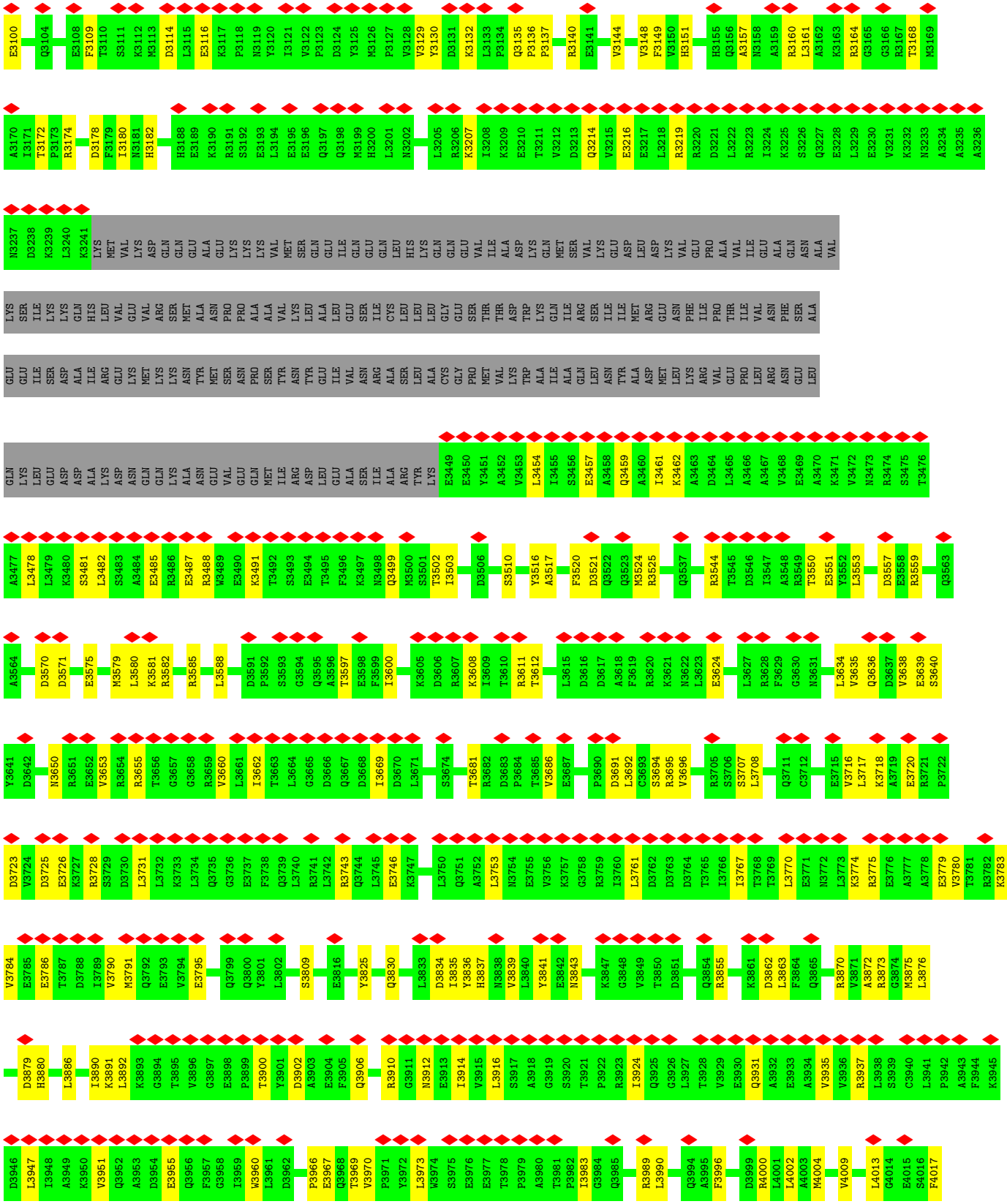
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N3237 D3238 K3239 L3240 K3241 LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLN GLU VAL ILE ALA ASP LYS GLN MET SER VAL LYS GLU ASP LEU ASP LYS VAL GLU PRO ALA VAL ILE GLU ALA GLN ASN ALA VAL
LYS SER ILE LYS LYS GLN HIS LEU VAL GLU VAL ARG SER MET ALA ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU SER ILE CYS LEU LEU LEU GLY GLU SER THR THR ASP TRP LYS GLN ILE ARG SER ILE ILE MET ARG GLU ASN PHE ILE PRO THR ILE 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 A3467 V3468 E3469 A3470 K3471 V3472 N3473 R3474 S3475 T3476
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Y3641 D3642 N3650 R3651 E3652 V3653 R3654 R3655 T3656 G3657 G3658 R3659 V3660 L3661 I3662 T3663 L3664 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 S3674 T3681 R3682 D3683 P3684 T3685 V3686 E3687 P3690 D3691 L3692 C3693 S3694 R3695 V3696 R3705 S3706 S3707 L3708 Q3711 C3712 E3715 V3716 L3717 K3718 A3719 E3720 R3721 P3722
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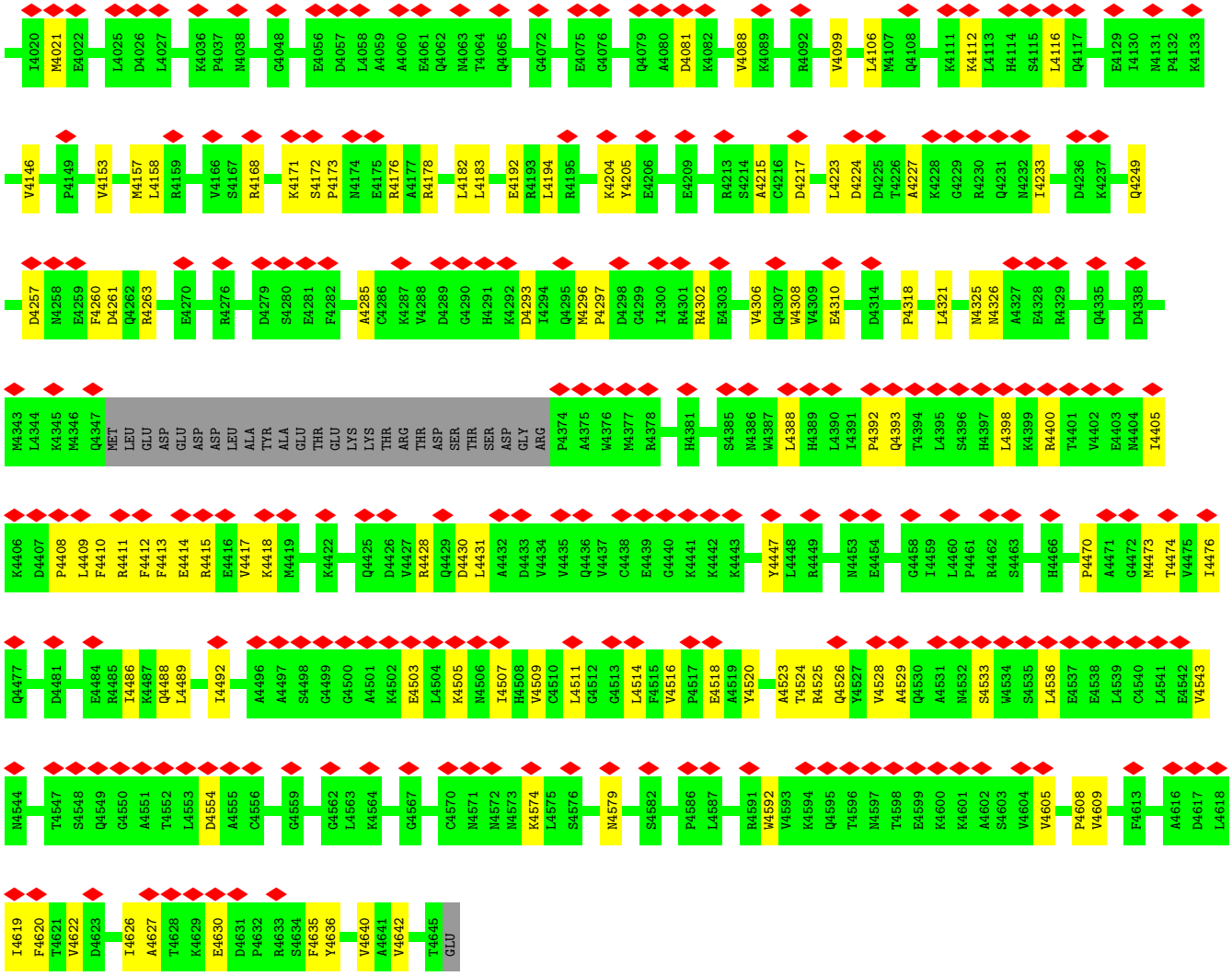
V3784 E3785 E3786 T3787 D3788 I3789 V3790 M3791 Q3792 E3793 V3794 E3795 Q3799 Q3800 Y3801 L3802 S3809 E3816 Y3825 Q3830 L3833 D3834 I3835 Y3836 H3837 N3838 V3839 L3840 Y3841 E3842 N3843 K3847 G3848 V3849 T3850 D3851 Q3854 R3855 K3861 D3862 L3863 F3864 Q3865 R3870 V3871 A3872 R3873 G3874 M3875 L3876
D3879 H3880 L3886 I3890 K3891 L3892 K3893 G3894 T3895 V3896 G3897 E3898 P3899 T3900 Y3901 D3902 A3903 E3904 F3905 Q3906 R3910 G3911 N3912 E3913 I3914 V3915 L3916 S3917 A3918 G3919 S3920 T3921 P3922 R3923 I3924 Q3925 G3926 L3927 T3928 V3929 E3930 Q3931 A3932 E3933 A3934 V3935 V3936 R3937 L3938 S3939 C3940 L3941 P3942 A3943 F3944 K3945
D3946 L3947 I3948 A3949 K3950 V3951 Q3952 A3953 D3964 E3955 Q3956 F3957 G3958 I3959 W3960 L3961 D3962 P3966 E3967 Q3968 T3969 V3970 P3971 Y3972 L3973 W3974 S3975 E3976 E3977 T3978 P3979 A3980 T3981 P3982 I3983 G3984 Q3985 R3989 L3990 Q3994 A3995 F3996 D3999 R4000 L4001 L4002 A4003 M4004 V4009 L4013 G4014 E4015 S4016 F4017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V4146 P4149 V4153 M4157 L4158 R4159 V4166 S4167 R4168 K4171 S4172 P4173 N4174 E4175 R4176 A4177 R4178 L4182 L4183 E4192 R4193 L4194 R4195 K4204 Y4205 E4206 E4209 R4213 S4214 A4215 G4216 D4217 L4223 D4224 D4225 T4226 A4227 K4228 G4229 R4230 Q4231 N4232 I4233 D4236 K4237 Q4249
D4257 N4258 E4259 F4260 D4261 Q4262 R4263 E4270 R4276 D4279 S4280 E4281 F4282 A4285 C4286 K4287 V4288 D4289 G4290 H4291 K4292 D4293 I4294 Q4295 M4296 P4297 D4298 G4299 I4300 R4301 R4302 E4303 V4306 Q4307 W4308 V4309 E4310 D4314 P4318 L4321 N4325 N4326 A4327 E4328 R4329 Q4335 D4338
M4343 L4344 K4345 M4346 Q4347 MET LEU GLU 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 M4377 R4378 H4381 S4385 N4386 W4387 L4388 H4389 L4390 I4391 P4392 Q4393 T4394 L4395 S4396 H4397 L4398 K4399 R4400 T4401 V4402 E4403 N4404 I4405
K4406 D4407 P4408 L4409 F4410 R4411 F4412 F4413 E4414 R4415 E4416 V4417 K4418 M4419 K4422 Q4425 D4426 V4427 R4428 Q4429 D4430 L4431 A4432 D4433 V4434 V4435 Q4436 V4437 C4438 E4439 G4440 K4441 K4442 K4443 Y4447 L4448 R4449 N4453 E4454 G4458 I4459 L4460 P4461 R4462 S4463 H4466 P4470 A4471 G4472 M4473 T4474 V4475 I4476
Q4477 D4481 E4484 R4485 I4486 K4487 Q4488 L4489 I4492 A4496 A4497 S4498 G4499 G4500 A4501 K4502 E4503 L4504 K4505 N4506 I4507 H4508 V4509 C4510 L4511 G4512 G4513 L4514 F4515 V4516 P4517 E4518 A4519 Y4520 A4523 T4524 R4525 Q4526 Y4527 V4528 A4529 Q4530 A4531 N4532 S4533 W4534 S4535 L4536 E4537 E4538 L4539 C4540 L4541 E4542 V4543
N4544 T4547 S4548 Q4549 G4550 A4551 T4552 L4553 D4554 A4555 C4556 G4559 G4562 L4563 K4564 G4567 C4570 N4571 N4572 N4573 K4574 L4575 S4576 N4579 S4582 P4586 L4587 R4591 W4592 V4593 K4594 Q4595 T4596 N4597 T4598 E4599 K4600 K4601 A4602 S4603 V4604 V4605 P4608 V4609 F4613 A4616 D4617 L4618
I4619 F4620 T4621 V4622 D4623 I4626 A4627 T4628 K4629 E4630 D4631 P4632 R4633 S4634 F4635 Y4636 V4640 A4641 V4642 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47152	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	1.222	Depositor
Minimum map value	-0.580	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.4	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	0.12	0/24075	0.28	0/32628

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	23575	0	23639	376	0
2	A	81	0	36	5	0
3	A	31	0	12	0	0
4	A	2	0	0	0	0
All	All	23689	0	23687	376	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 8.

All (376) 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:1497:VAL:HG13	1:A:1527:LEU:HD22	1.59	0.85
1:A:2156:LEU:HG	1:A:4411:ARG:HD2	1.59	0.83
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.62	0.81
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.65	0.79
1:A:1810:HIS:HD2	1:A:1878:LYS:HG3	1.48	0.78
1:A:2092:ALA:HB1	1:A:2145:MET:HE1	1.64	0.78
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.67	0.77
1:A:4260:PHE:HD1	1:A:4263:ARG:HH21	1.36	0.74
1:A:1526:LYS:HA	1:A:1529:ARG:HD3	1.68	0.74
1:A:3488:ARG:NH2	1:A:3746:GLU:OE1	2.21	0.74
1:A:3502:THR:HG21	1:A:3544:ARG:HG3	1.70	0.73
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.21	0.73
1:A:1652:LYS:HG3	1:A:1653:HIS:HD2	1.52	0.73
1:A:4413:PHE:CZ	1:A:4492:ILE:HG23	2.24	0.72
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.71	0.72
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.71	0.71
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.72	0.71
1:A:1523:TRP:HA	1:A:1526:LYS:HE3	1.73	0.69
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.74	0.69
1:A:4393:GLN:HG3	1:A:4428:ARG:HH12	1.58	0.68
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.74	0.68
1:A:1806:ARG:O	1:A:1810:HIS:ND1	2.21	0.68
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.27	0.68
1:A:3487:GLU:OE1	1:A:3491:LYS:NZ	2.27	0.67
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	1.78	0.65
1:A:3078:ARG:HA	1:A:3081:THR:HG22	1.78	0.65
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.30	0.65
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.77	0.64
1:A:3481:SER:O	1:A:3774:LYS:NZ	2.30	0.64
1:A:3731:LEU:HD21	1:A:3790:VAL:HB	1.80	0.64
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.31	0.63
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.78	0.63
1:A:3499:GLN:O	1:A:3503:ILE:HG13	1.99	0.62
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.79	0.62
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.63	0.62
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.65	0.62
1:A:2382:LEU:HD12	1:A:2416:GLN:HE21	1.65	0.62
1:A:2485:GLN:OE1	1:A:2488:ARG:NH2	2.32	0.62
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.35	0.62
1:A:2172:ARG:NH1	1:A:2205:GLU:OE2	2.33	0.62
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.83	0.61
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.81	0.61
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.83	0.61
1:A:2172:ARG:NH2	1:A:2212:GLN:OE1	2.35	0.60
1:A:1543:ARG:HA	1:A:1546:TYR:CE1	2.37	0.60
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.83	0.60
1:A:1504:VAL:HG11	1:A:1524:GLU:HG3	1.84	0.60
1:A:2080:LEU:HD23	1:A:2156:LEU:HD22	1.83	0.59
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.82	0.59
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.82	0.59
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.35	0.59
1:A:1652:LYS:HG3	1:A:1653:HIS:CD2	2.36	0.59
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.36	0.59
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.20	0.59
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.84	0.59
1:A:1943:ARG:NH1	1:A:2329:ASN:O	2.36	0.59
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.85	0.59
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.34	0.59
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.68	0.59
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.85	0.58
1:A:1639:GLU:OE2	1:A:1643:ASN:ND2	2.36	0.58
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.85	0.58
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.37	0.58
1:A:3478:LEU:HD22	1:A:3767:ILE:HG23	1.86	0.58
1:A:2410:SER:HB3	1:A:2413:LEU:HD23	1.87	0.57
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.83	0.57
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.85	0.57
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.36	0.57
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.38	0.57
1:A:3581:LYS:HE3	1:A:3582:ARG:HG3	1.86	0.57
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.87	0.57
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.36	0.57
1:A:2864:GLU:OE1	1:A:2864:GLU:N	2.36	0.57
1:A:2094:LYS:NZ	2:A:4701:ADP:O2'	2.34	0.57
1:A:2519:ARG:HG3	1:A:2526:LEU:HD22	1.86	0.57
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.86	0.57
1:A:3779:GLU:O	1:A:3783:LYS:HG2	2.04	0.57
1:A:3482:LEU:HD11	1:A:3770:LEU:HD23	1.86	0.56
1:A:1887:ARG:HD2	1:A:4249:GLN:HG2	1.87	0.56
1:A:1987:ASN:OD1	1:A:1989:ASN:ND2	2.38	0.56
1:A:4525:ARG:HD3	1:A:4536:LEU:HD23	1.88	0.56
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.39	0.55
1:A:1589:MET:SD	1:A:1589:MET:N	2.80	0.55
1:A:3875:MET:HE3	1:A:3880:HIS:HA	1.88	0.55
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.40	0.55
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.35	0.55
1:A:1763:GLU:OE1	1:A:1838:TRP:NE1	2.34	0.54
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.71	0.54
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.88	0.54
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.36	0.54
1:A:3967:GLU:HB2	1:A:4004:MET:HE2	1.88	0.54
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.88	0.54
1:A:3960:TRP:HD1	1:A:3969:THR:HG23	1.72	0.54
1:A:4489:LEU:HD23	1:A:4492:ILE:HD12	1.88	0.54
1:A:2080:LEU:HD11	1:A:2157:LEU:HD12	1.89	0.54
1:A:3459:GLN:HA	1:A:3462:LYS:HD2	1.89	0.54
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.90	0.54
1:A:4518:GLU:OE1	1:A:4518:GLU:N	2.33	0.54
1:A:4398:LEU:HD12	1:A:4414:GLU:HA	1.89	0.53
1:A:2694:ARG:NH2	1:A:2697:ASP:OD2	2.39	0.53
1:A:4409:LEU:O	1:A:4413:PHE:HB2	2.08	0.53
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.41	0.53
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.43	0.53
1:A:3653:VAL:HG12	1:A:3662:ILE:HB	1.88	0.53
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.90	0.53
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.90	0.53
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.26	0.53
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.91	0.52
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.91	0.52
1:A:4194:LEU:HD11	1:A:4204:LYS:HA	1.91	0.52
1:A:4605:VAL:HG23	1:A:4636:TYR:HE1	1.75	0.52
1:A:2495:VAL:HG21	1:A:2524:VAL:HG21	1.90	0.52
1:A:3216:GLU:HG2	1:A:3219:ARG:HH21	1.74	0.52
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.91	0.52
1:A:2654:GLN:NE2	1:A:3048:GLU:OE2	2.43	0.52
1:A:4474:THR:HG22	1:A:4476:ILE:H	1.75	0.52
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.58	0.51
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.93	0.51
1:A:2363:TRP:NE1	1:A:2365:SER:OG	2.43	0.51
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.09	0.51
1:A:2440:ALA:HB2	1:A:2502:LEU:HD23	1.92	0.51
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.11	0.51
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.92	0.51
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.93	0.51
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.93	0.51
1:A:1847:ASP:N	1:A:1856:GLN:O	2.41	0.51
1:A:3130:TYR:CZ	1:A:3132:LYS:HB3	2.45	0.51
1:A:3720:GLU:OE1	1:A:3855:ARG:NE	2.43	0.51
1:A:4081:ASP:OD1	1:A:4112:LYS:NZ	2.44	0.51
1:A:1527:LEU:HD23	1:A:1530:ILE:HD12	1.92	0.50
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.23	0.50
1:A:3160:ARG:HE	1:A:3164:ARG:HH21	1.60	0.50
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.93	0.50
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.44	0.50
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.28	0.50
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.92	0.50
1:A:2481:MET:HE2	1:A:2485:GLN:HB3	1.94	0.50
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.94	0.50
1:A:4021:MET:HA	1:A:4021:MET:HE2	1.94	0.50
1:A:4408:PRO:HG3	1:A:4526:GLN:HB3	1.92	0.50
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.75	0.50
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.11	0.50
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.93	0.50
1:A:1941:MET:HE3	1:A:1971:VAL:HG11	1.94	0.49
1:A:1535:ASP:O	1:A:2292:ARG:NH2	2.45	0.49
1:A:2485:GLN:NE2	1:A:2542:SER:O	2.45	0.49
1:A:2507:ARG:HH22	1:A:2510:MET:HE2	1.78	0.49
1:A:4392:PRO:O	1:A:4428:ARG:NH1	2.45	0.49
1:A:4192:GLU:HB2	1:A:4321:LEU:HD21	1.95	0.49
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.95	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.13	0.49
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.47	0.49
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.13	0.49
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.93	0.49
1:A:3144:VAL:O	1:A:3148:VAL:HG23	2.13	0.48
1:A:4153:VAL:O	1:A:4157:MET:HG3	2.13	0.48
1:A:3639:GLU:OE2	1:A:3681:THR:OG1	2.30	0.48
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.14	0.48
1:A:2291:VAL:HG13	1:A:2292:ARG:HG3	1.95	0.48
1:A:3775:ARG:O	1:A:3779:GLU:HG2	2.12	0.48
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.14	0.48
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3160:ARG:HE	1:A:3164:ARG:NH2	2.11	0.48
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.46	0.48
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.41	0.48
1:A:4525:ARG:HG3	1:A:4592:TRP:CH2	2.48	0.48
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.46	0.48
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.47	0.48
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	1.94	0.48
1:A:3030:MET:HA	1:A:3030:MET:HE3	1.96	0.48
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.95	0.47
1:A:1980:GLU:O	1:A:1984:GLU:HG2	2.14	0.47
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	1.96	0.47
1:A:1912:LYS:NZ	2:A:4701:ADP:O3B	2.33	0.47
1:A:1985:HIS:CE1	1:A:2010:PRO:HG3	2.49	0.47
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.48	0.47
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.94	0.47
1:A:2605:LEU:HD13	1:A:2709:VAL:HG11	1.96	0.47
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.14	0.47
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.96	0.47
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.97	0.47
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.14	0.47
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	1.96	0.47
1:A:3872:ALA:HA	1:A:3875:MET:HE2	1.97	0.47
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.31	0.47
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.97	0.47
1:A:2463:HIS:O	1:A:2467:ARG:HG3	2.14	0.47
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.14	0.47
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.25	0.47
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.48	0.47
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.30	0.47
1:A:4509:VAL:HG11	1:A:4514:LEU:HD11	1.96	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.50	0.47
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.33	0.47
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	1.96	0.47
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.48	0.47
1:A:3960:TRP:CD1	1:A:3969:THR:HG23	2.49	0.47
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.97	0.47
1:A:2075:LEU:HD13	1:A:2160:LEU:HD11	1.96	0.46
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.48	0.46
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.16	0.46
1:A:4413:PHE:O	1:A:4417:VAL:HG23	2.14	0.46
1:A:1738:TYR:CE2	1:A:1792:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3109:PHE:HD2	1:A:3180:ILE:HG22	1.80	0.46
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.15	0.46
1:A:3728:ARG:HG3	1:A:3791:MET:HE1	1.97	0.46
1:A:4408:PRO:HB3	1:A:4411:ARG:HH21	1.79	0.46
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	1.97	0.46
1:A:3791:MET:O	1:A:3795:GLU:HG3	2.14	0.46
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.49	0.46
1:A:1490:TRP:HZ3	1:A:1534:PHE:HD1	1.64	0.46
1:A:1903:SER:HA	1:A:2016:ILE:O	2.15	0.46
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.98	0.46
1:A:1467:ARG:HB2	1:A:1523:TRP:HH2	1.80	0.46
1:A:1550:ILE:O	1:A:1554:SER:OG	2.29	0.46
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.98	0.46
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.98	0.46
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.81	0.46
1:A:2446:ILE:HG13	1:A:2735:TYR:CD1	2.51	0.46
1:A:1508:LYS:HA	1:A:1513:TYR:CG	2.51	0.45
1:A:3100:GLU:HG2	1:A:3130:TYR:HE1	1.80	0.45
1:A:2983:SER:HB2	1:A:2990:ILE:HD12	1.99	0.45
1:A:4412:PHE:HE1	1:A:4516:VAL:HG23	1.81	0.45
1:A:2606:PHE:HE1	1:A:2617:VAL:HG21	1.81	0.45
1:A:2018:MET:HE2	1:A:2018:MET:HB3	1.88	0.45
1:A:2885:ASP:HB3	1:A:2888:GLU:OE1	2.16	0.45
1:A:4412:PHE:CZ	1:A:4514:LEU:HD13	2.51	0.45
1:A:2104:LYS:HG3	1:A:2131:LEU:HD21	1.99	0.45
1:A:3843:ASN:ND2	1:A:3862:ASP:OD2	2.48	0.45
1:A:4410:PHE:HA	1:A:4413:PHE:HB3	1.99	0.45
1:A:2624:SER:HB3	1:A:3081:THR:HA	1.98	0.45
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.17	0.45
1:A:2901:TYR:CZ	1:A:2908:PRO:HA	2.50	0.45
1:A:4409:LEU:HA	1:A:4523:ALA:HB1	1.99	0.45
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.98	0.45
1:A:1507:MET:O	1:A:1510:SER:OG	2.29	0.45
1:A:1526:LYS:O	1:A:1530:ILE:HG13	2.17	0.45
1:A:2257:LYS:HZ3	1:A:2308:ASP:CG	2.24	0.45
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.17	0.45
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.48	0.45
1:A:2103:VAL:HA	1:A:2106:GLU:HG2	1.99	0.45
1:A:3551:GLU:HA	1:A:3559:ARG:NH1	2.32	0.45
1:A:4489:LEU:HA	1:A:4492:ILE:HD12	1.98	0.45
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2671:MET:HE2	1:A:2675:GLY:HA2	1.99	0.45
1:A:1640:ILE:HA	1:A:1650:LEU:HD22	2.00	0.44
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.17	0.44
1:A:3837:HIS:CE1	1:A:3841:TYR:HD2	2.35	0.44
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.53	0.44
1:A:2965:ARG:HH12	1:A:3640:SER:HB3	1.81	0.44
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.33	0.44
1:A:1572:SER:O	1:A:1576:LEU:HG	2.18	0.44
1:A:2324:LEU:HD23	1:A:2334:SER:HA	1.99	0.44
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.53	0.44
1:A:2571:THR:O	1:A:2575:VAL:HG22	2.16	0.44
1:A:4488:GLN:O	1:A:4492:ILE:HG13	2.18	0.44
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.99	0.44
1:A:4400:ARG:HD2	1:A:4405:ILE:HD11	1.98	0.44
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	2.00	0.44
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.51	0.44
1:A:1568:PHE:HB2	1:A:1611:ILE:HD13	1.99	0.43
1:A:2949:PHE:CZ	1:A:2953:MET:HE3	2.53	0.43
1:A:1623:ARG:HA	1:A:1629:PHE:HB2	2.01	0.43
1:A:2159:SER:OG	1:A:4411:ARG:NH1	2.52	0.43
1:A:2527:PRO:HD3	1:A:2545:TRP:CD2	2.54	0.43
1:A:2816:LEU:HD21	1:A:2821:LEU:N	2.33	0.43
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	2.00	0.43
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	2.00	0.43
1:A:1960:PHE:HE2	1:A:2032:LEU:HD21	1.82	0.43
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.19	0.43
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.18	0.43
1:A:4626:ILE:HD12	1:A:4630:GLU:O	2.18	0.43
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.45	0.43
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	2.00	0.43
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.86	0.43
1:A:1558:LYS:HD3	1:A:1565:THR:HG21	2.00	0.43
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.54	0.43
1:A:4182:LEU:HG	1:A:4296:MET:HE1	2.01	0.43
1:A:4525:ARG:HG3	1:A:4592:TRP:CZ3	2.54	0.43
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.18	0.43
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.18	0.43
1:A:3597:THR:HG21	1:A:3611:ARG:HH12	1.84	0.43
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.81	0.43
1:A:1738:TYR:HE2	1:A:1792:LEU:HD11	1.83	0.43
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1542:ARG:O	1:A:1546:TYR:HD1	2.02	0.43
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	2.01	0.43
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	2.01	0.42
1:A:2507:ARG:HH21	1:A:2509:LYS:HE2	1.83	0.42
1:A:2936:ILE:O	1:A:3094:PHE:N	2.52	0.42
1:A:4630:GLU:HB3	1:A:4635:PHE:HE1	1.84	0.42
1:A:1933:ASP:OD1	1:A:1935:THR:HG22	2.19	0.42
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.44	0.42
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	2.00	0.42
1:A:3207:LYS:HD3	1:A:3207:LYS:HA	1.85	0.42
1:A:3214:GLN:HB3	1:A:3761:LEU:HD12	2.00	0.42
1:A:3951:VAL:HG12	1:A:3973:LEU:HD21	2.00	0.42
1:A:1543:ARG:HA	1:A:1546:TYR:CD1	2.55	0.42
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	2.00	0.42
1:A:2308:ASP:OD1	1:A:2311:TRP:HD1	2.03	0.42
1:A:2386:PRO:HG3	1:A:2413:LEU:HD21	2.00	0.42
1:A:3900:THR:HG23	1:A:3902:ASP:H	1.84	0.42
1:A:1814:GLU:OE1	1:A:1878:LYS:NZ	2.52	0.42
1:A:3457:GLU:O	1:A:3461:ILE:HG12	2.19	0.42
1:A:4529:ALA:O	1:A:4533:SER:N	2.53	0.42
1:A:1879:LEU:HD22	2:A:4701:ADP:C4	2.55	0.42
1:A:3039:LYS:HB3	1:A:3039:LYS:HE3	1.78	0.42
1:A:3906:GLN:NE2	1:A:3910:ARG:HD2	2.34	0.42
1:A:4470:PRO:HD2	1:A:4473:MET:HE3	2.02	0.42
1:A:2083:GLN:HE21	1:A:2150:VAL:HG11	1.85	0.42
1:A:3454:LEU:O	1:A:3457:GLU:HG2	2.20	0.42
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.47	0.42
1:A:1561:LEU:HB3	1:A:1564:GLU:OE2	2.19	0.42
1:A:1587:LEU:HD12	1:A:1587:LEU:HA	1.94	0.41
1:A:1680:GLU:HG2	1:A:1803:LEU:HD13	2.02	0.41
1:A:2163:ASP:HB3	1:A:4526:GLN:HE21	1.84	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.54	0.41
1:A:2686:MET:HE3	1:A:2708:PHE:CZ	2.54	0.41
1:A:4486:ILE:HD13	1:A:4486:ILE:HA	1.90	0.41
1:A:1501:ILE:HG13	1:A:1527:LEU:HD13	2.01	0.41
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.53	0.41
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.85	0.41
1:A:4400:ARG:NE	1:A:4414:GLU:OE1	2.53	0.41
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	2.02	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.03	0.41
1:A:2313:GLU:OE2	1:A:2352:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3085:LEU:O	1:A:3089:CYS:HB2	2.21	0.41
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	2.03	0.41
1:A:1814:GLU:O	1:A:1818:GLN:HG3	2.21	0.41
1:A:1969:SER:O	1:A:1972:SER:OG	2.35	0.41
1:A:2091:ARG:HH21	2:A:4701:ADP:PA	2.44	0.41
1:A:2766:ALA:O	1:A:2770:THR:HG22	2.21	0.41
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.21	0.41
1:A:1645:LYS:HA	1:A:1645:LYS:HD2	1.77	0.41
1:A:3608:LYS:HD2	1:A:3608:LYS:HA	1.67	0.41
1:A:2671:MET:HA	1:A:2676:THR:O	2.19	0.41
1:A:2949:PHE:CE2	1:A:2953:MET:HE3	2.56	0.41
1:A:3955:GLU:OE1	1:A:3955:GLU:N	2.52	0.41
1:A:1672:VAL:HG22	1:A:1691:SER:HB3	2.03	0.41
1:A:1810:HIS:CD2	1:A:1878:LYS:HG3	2.39	0.41
1:A:2525:PRO:C	1:A:2526:LEU:HD12	2.45	0.41
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.45	0.41
1:A:2079:GLN:O	1:A:4415:ARG:NH1	2.47	0.41
1:A:2228:SER:HB2	1:A:2364:PHE:HB3	2.01	0.41
1:A:2541:ILE:HD12	1:A:2541:ILE:HA	1.95	0.41
1:A:3550:THR:HG22	1:A:3575:GLU:HG3	2.03	0.41
1:A:3723:ASP:O	1:A:3726:GLU:HG2	2.21	0.41
1:A:4260:PHE:CZ	1:A:4608:PRO:HB3	2.55	0.41
1:A:1749:LEU:HD23	1:A:1749:LEU:HA	1.86	0.41
1:A:3570:ASP:OD2	1:A:3707:SER:HB3	2.21	0.41
1:A:3612:THR:O	1:A:3635:VAL:HA	2.20	0.41
1:A:3718:LYS:HB2	1:A:3725:ASP:OD2	2.20	0.41
1:A:4285:ALA:O	1:A:4293:ASP:HB2	2.20	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:4418:LYS:HE3	1:A:4418:LYS:HB2	1.88	0.41
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.89	0.41
1:A:2697:ASP:N	1:A:2697:ASP:OD1	2.50	0.40
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.53	0.40
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.21	0.40
1:A:4002:LEU:HD23	1:A:4002:LEU:HA	1.92	0.40
1:A:3109:PHE:CD2	1:A:3180:ILE:HG22	2.56	0.40
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.94	0.40
1:A:1467:ARG:HB2	1:A:1523:TRP:CH2	2.57	0.40
1:A:1564:GLU:HA	1:A:1567:ARG:HB2	2.04	0.40
1:A:1941:MET:HE1	1:A:1960:PHE:HE1	1.86	0.40
1:A:2029:PRO:HB2	1:A:2031:ASN:OD1	2.22	0.40
1:A:2075:LEU:HB3	1:A:2160:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4158:LEU:HD21	1:A:4310:GLU:HG3	2.03	0.40
1:A:4605:VAL:HG23	1:A:4636:TYR:CE1	2.55	0.40
1:A:4635:PHE:HD2	1:A:4640:VAL:HG11	1.85	0.40
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.86	0.40
1:A:3485:GLU:HG3	1:A:3488:ARG:HH21	1.86	0.40
1:A:4172:SER:HB2	1:A:4173:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2927/4646 (63%)	2883 (98%)	44 (2%)	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	2603/4125 (63%)	2603 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1465	GLN
1	A	1612	GLN
1	A	1643	ASN
1	A	1653	HIS
1	A	1755	GLN
1	A	1856	GLN
1	A	1922	GLN
1	A	1976	GLN
1	A	1989	ASN
1	A	2057	GLN
1	A	2067	ASN
1	A	2171	HIS
1	A	2218	HIS
1	A	2416	GLN
1	A	2588	HIS
1	A	2752	ASN
1	A	2827	HIS
1	A	2960	GLN
1	A	3200	HIS
1	A	3237	ASN
1	A	3526	GLN
1	A	3711	GLN
1	A	3754	ASN
1	A	3799	GLN
1	A	3820	GLN
1	A	3838	ASN
1	A	4029	HIS
1	A	4054	HIS
1	A	4114	HIS
1	A	4156	ASN
1	A	4191	GLN
1	A	4307	GLN
1	A	4335	GLN
1	A	4429	GLN
1	A	4526	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	4703	-	24,29,29	0.86	0	29,45,45	1.20	2 (6%)
2	ADP	A	4701	4	24,29,29	0.86	0	29,45,45	1.23	2 (6%)
3	ATP	A	4702	4	28,33,33	0.67	0	34,52,52	0.59	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	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4701	4	-	0/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	7/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4703	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4701	ADP	N3-C2-N1	-3.61	123.77	128.67
2	A	4704	ADP	N3-C2-N1	-3.61	123.78	128.67
2	A	4704	ADP	C4-C5-N7	-2.57	106.62	109.34
2	A	4703	ADP	C4-C5-N7	-2.45	106.74	109.34
2	A	4701	ADP	C4-C5-N7	-2.43	106.77	109.34
3	A	4702	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

All (8) torsion outliers are listed below:

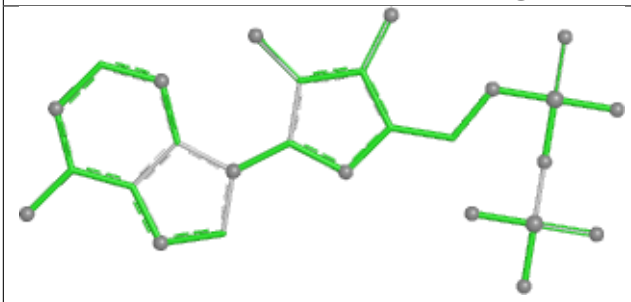
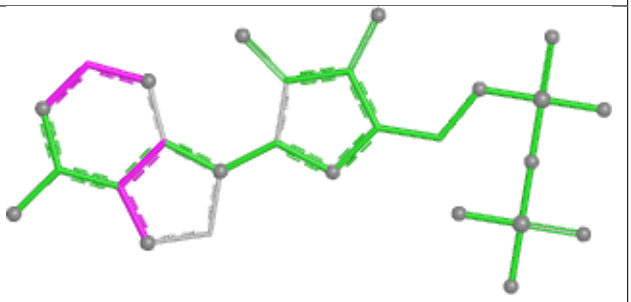
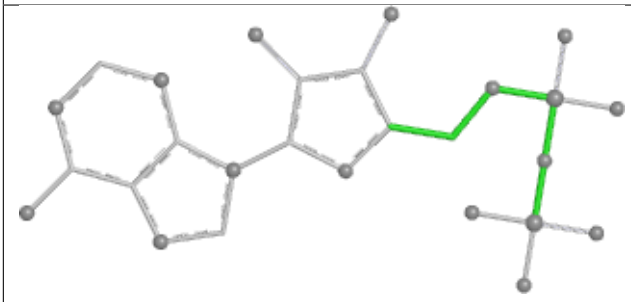
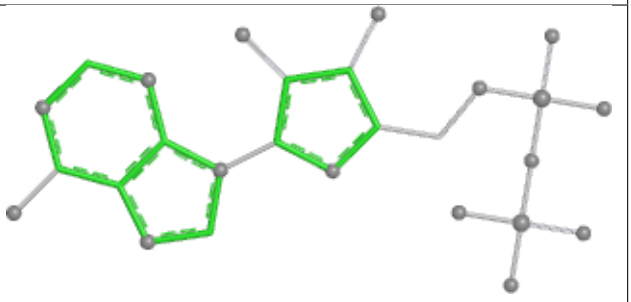
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O3A
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	PA-O3A-PB-O2B

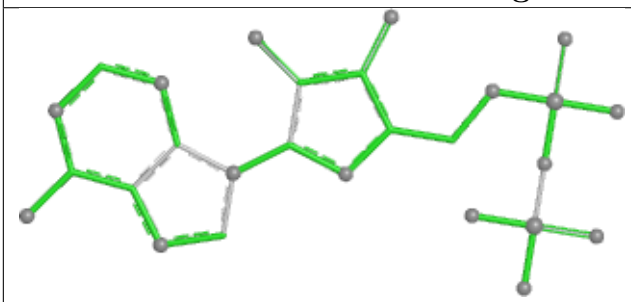
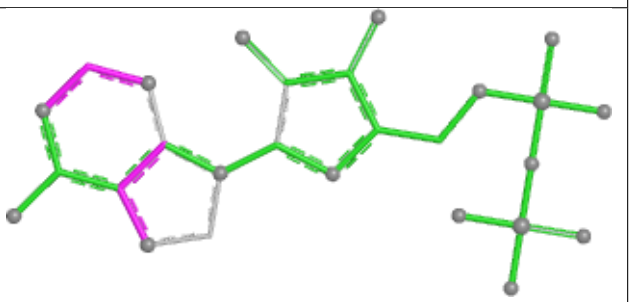
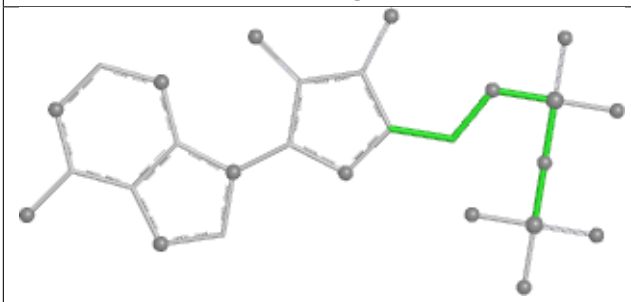
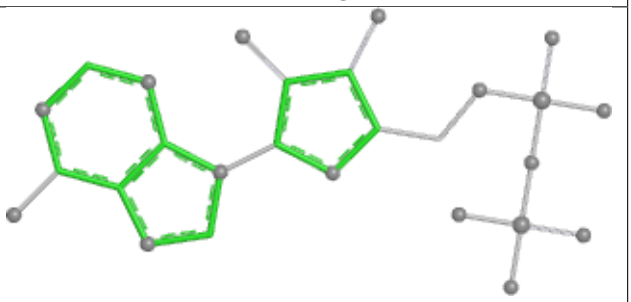
There are no ring outliers.

1 monomer is involved in 5 short contacts:

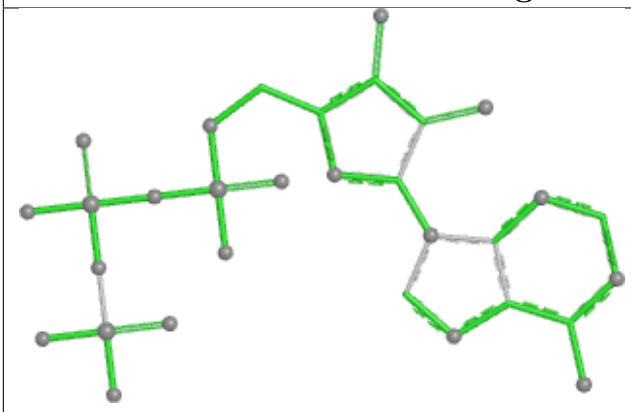
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	5	0

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.

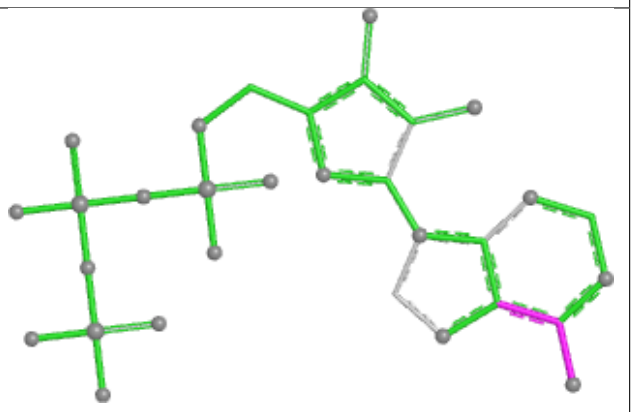
Ligand ADP A 4703	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 4701	
 Bond lengths	 Bond angles
 Torsions	 Rings

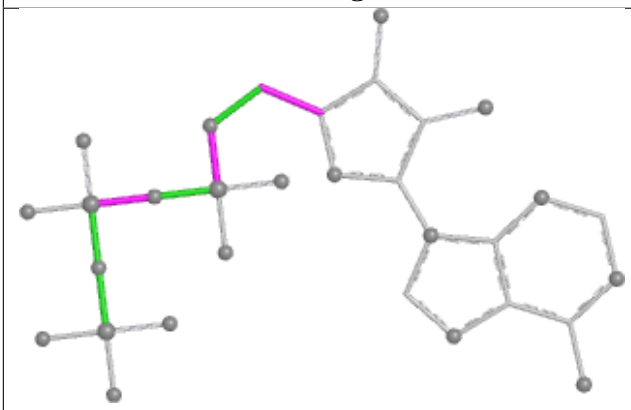
Ligand ATP A 4702



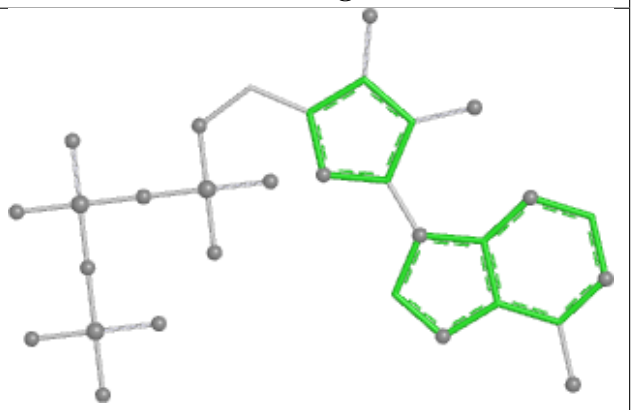
Bond lengths



Bond angles

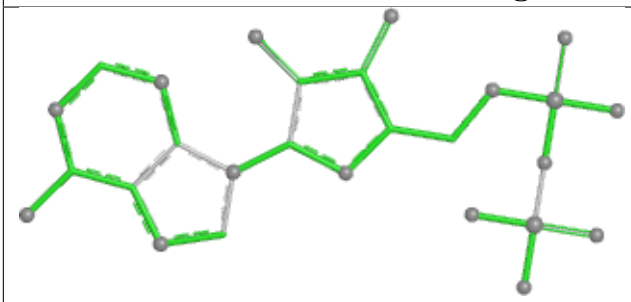


Torsions

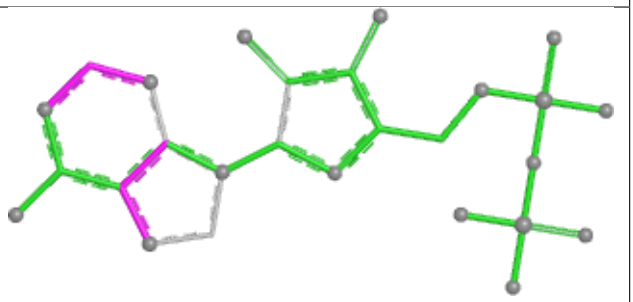


Rings

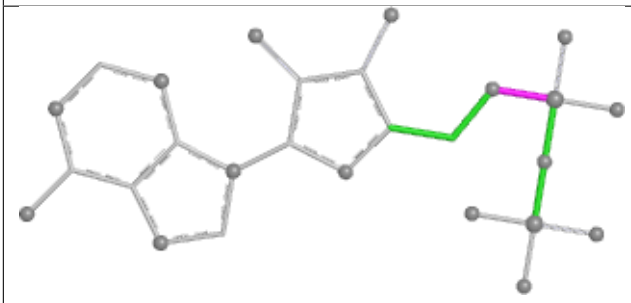
Ligand ADP A 4704



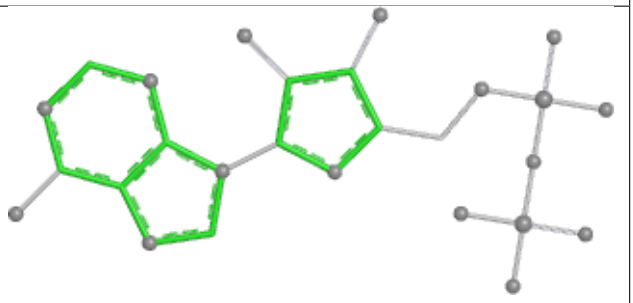
Bond lengths



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.

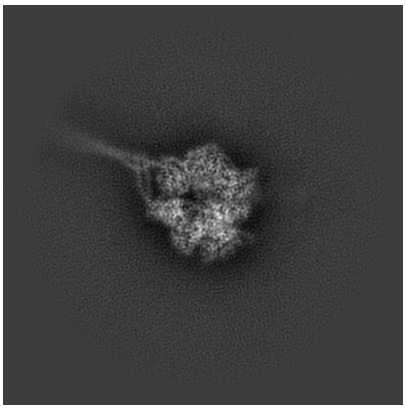
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46857. These allow visual inspection of the internal detail of the map and identification of artifacts.

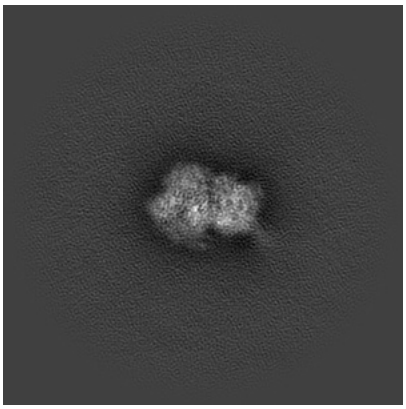
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

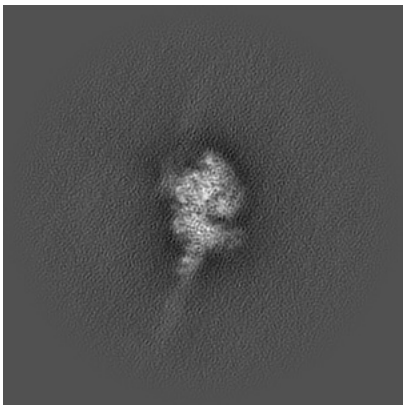
6.1.1 Primary map



X

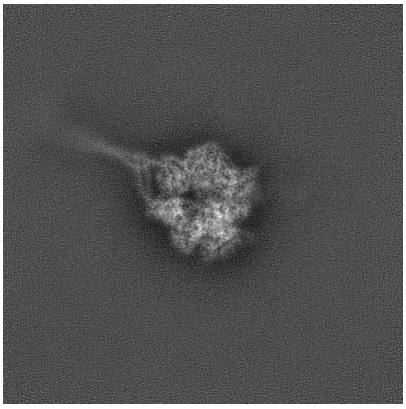


Y

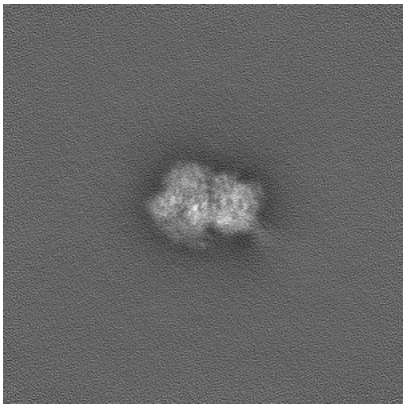


Z

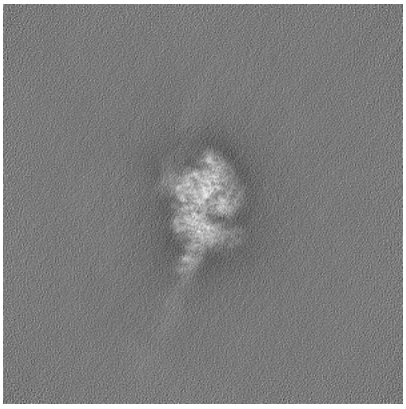
6.1.2 Raw map



X



Y

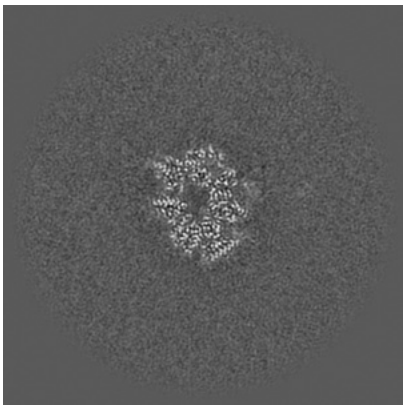


Z

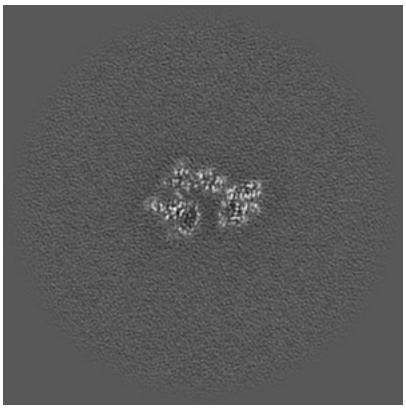
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

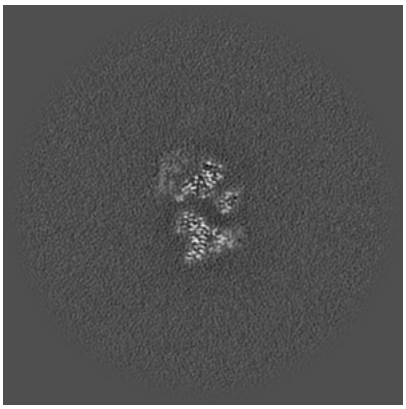
6.2.1 Primary map



X Index: 192

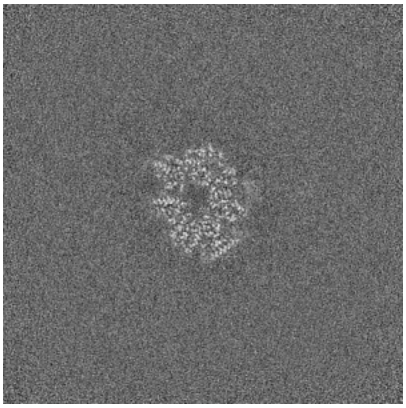


Y Index: 192

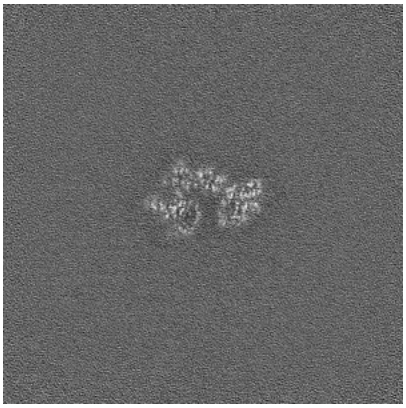


Z Index: 192

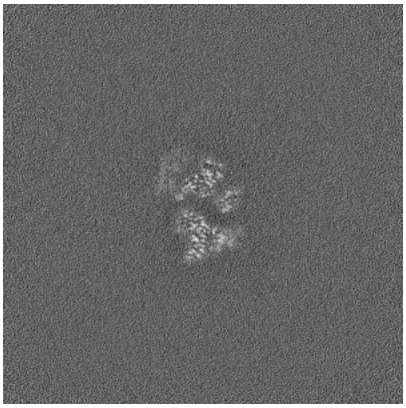
6.2.2 Raw map



X Index: 192



Y Index: 192

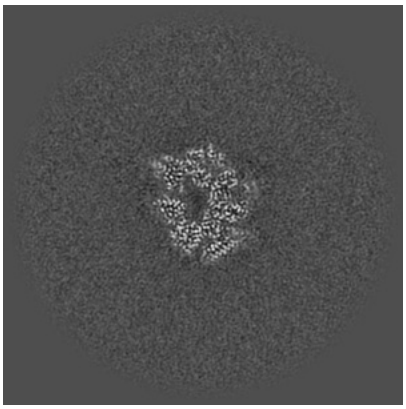


Z Index: 192

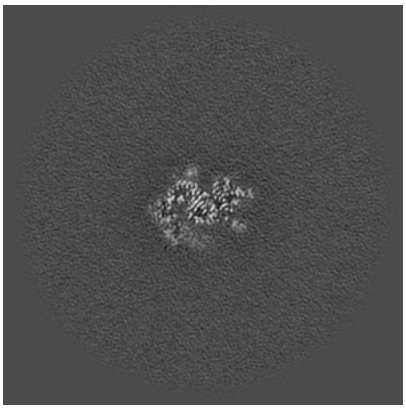
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

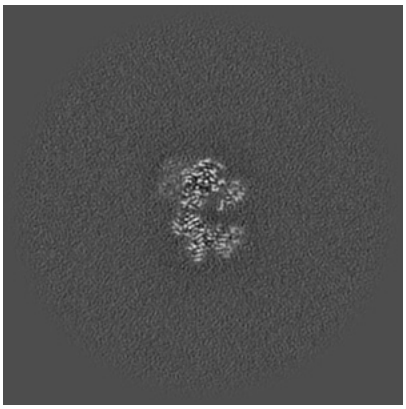
6.3.1 Primary map



X Index: 193

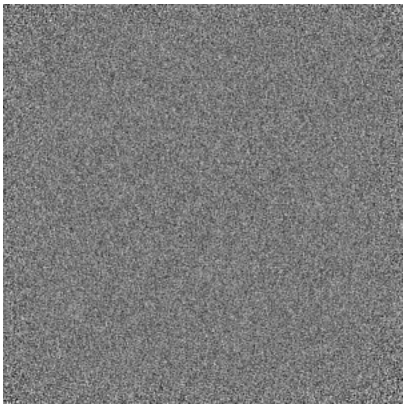


Y Index: 214

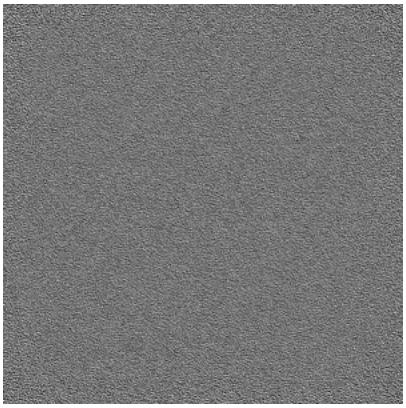


Z Index: 185

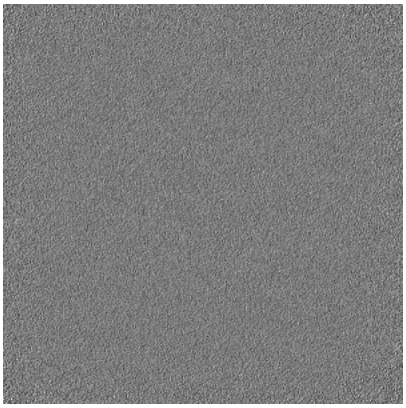
6.3.2 Raw map



X Index: 0



Y Index: 0

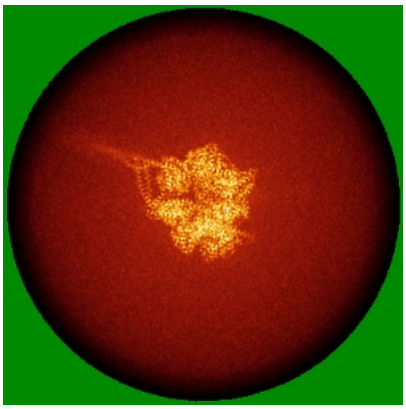


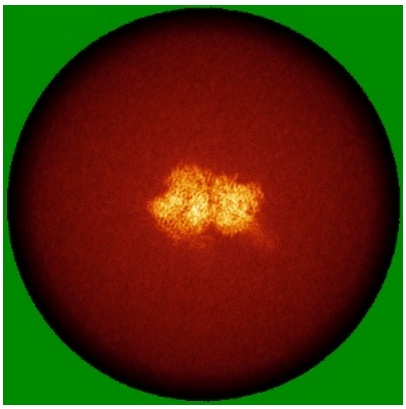
Z Index: 0

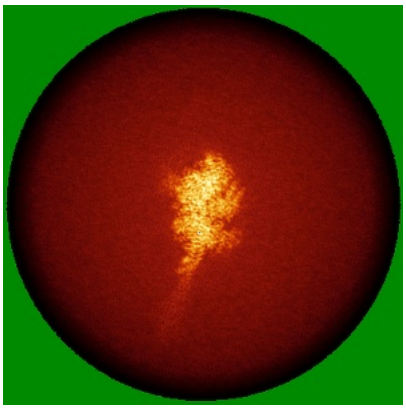
The images above show the largest variance slices of the map in three orthogonal directions.

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

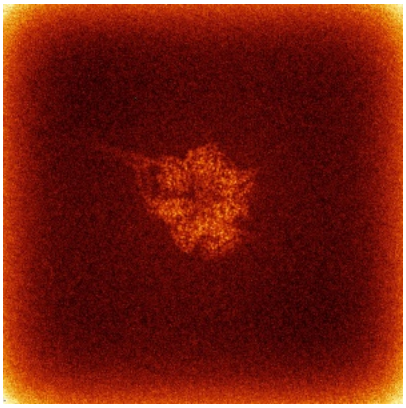
6.4.1 Primary map

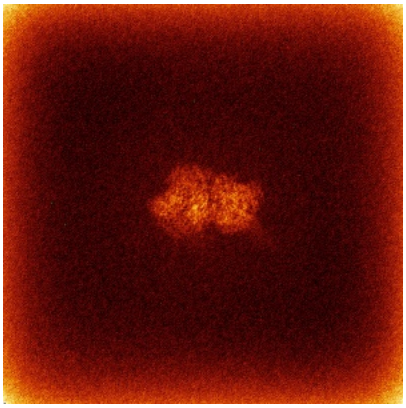

X

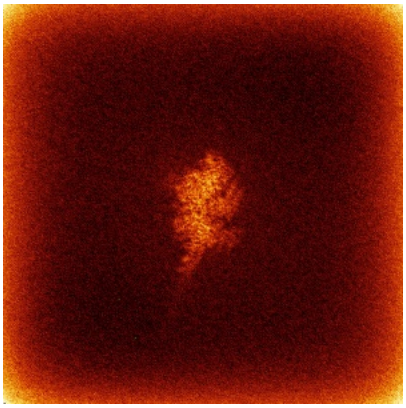

Y


Z

6.4.2 Raw map


X

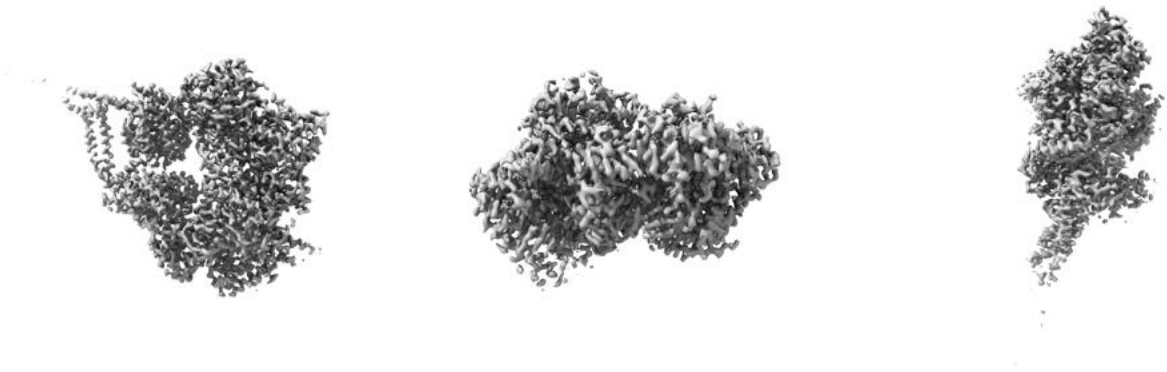

Y


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 0.4. 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.

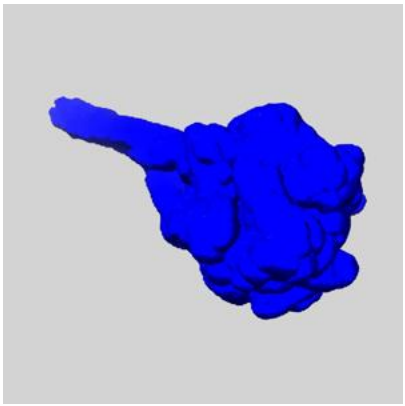
6.6 Mask visualisation (i)

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

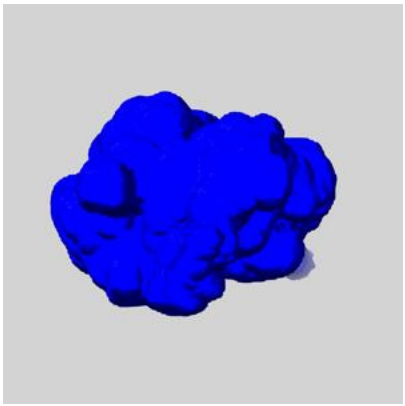
A mask typically either:

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

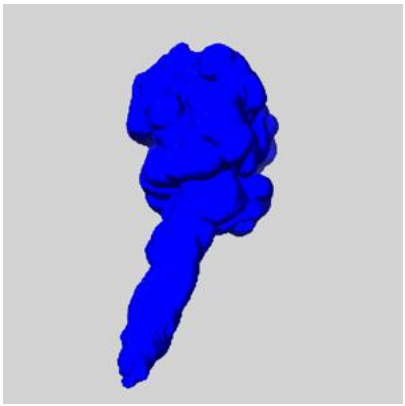
6.6.1 emd_46857_msk_1.map (i)



X



Y

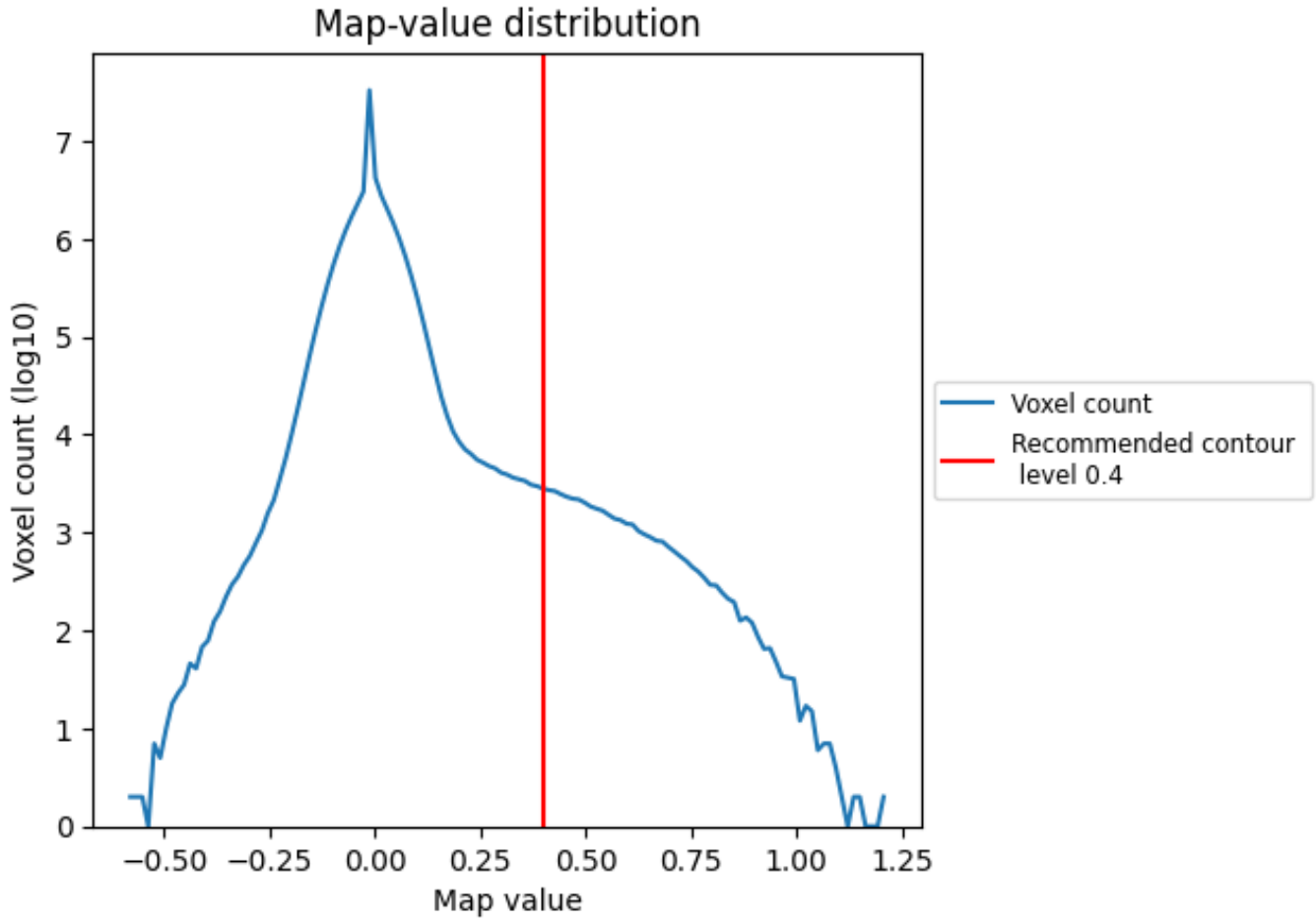


Z

7 Map analysis

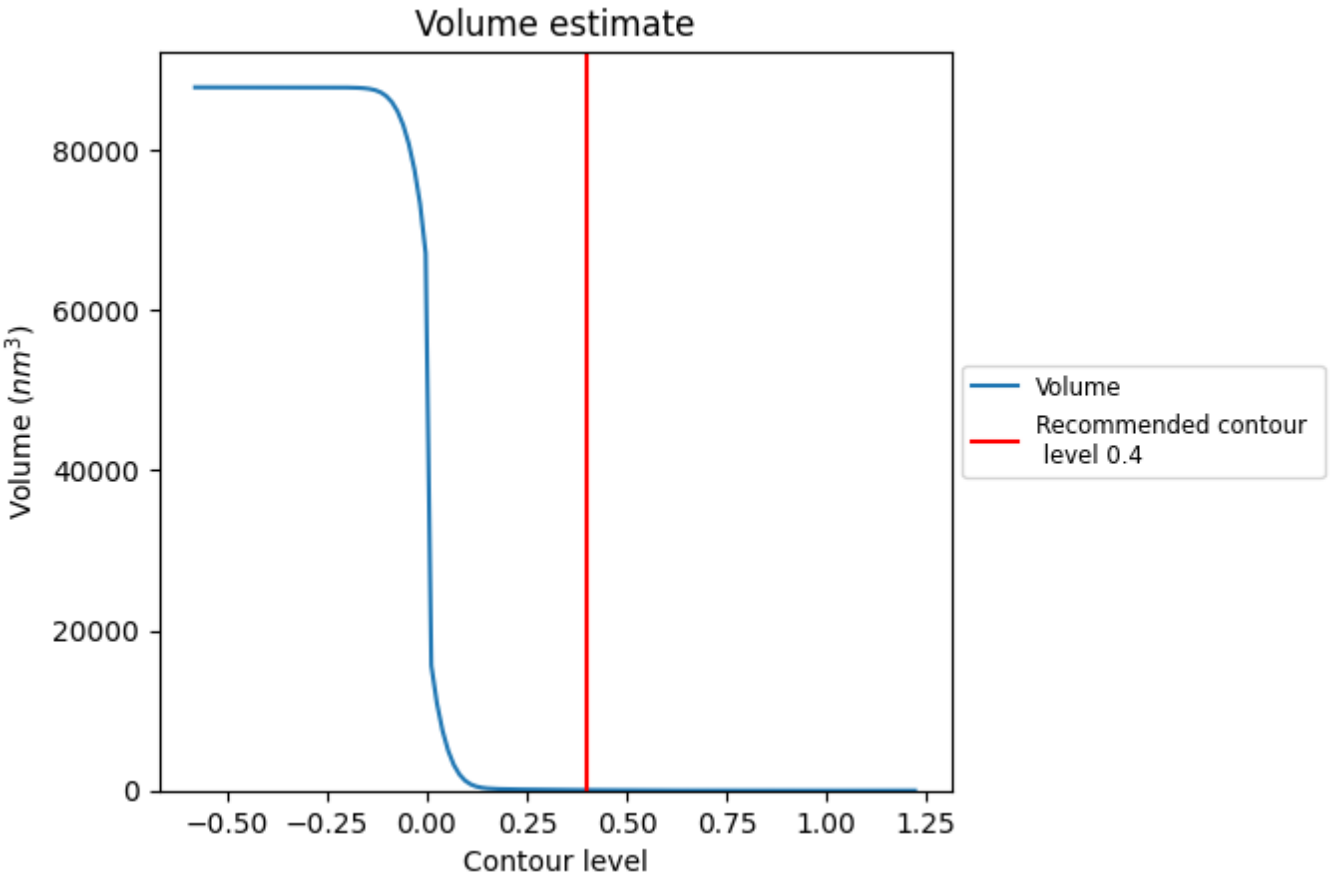
This section contains the results of statistical analysis of the map.

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.

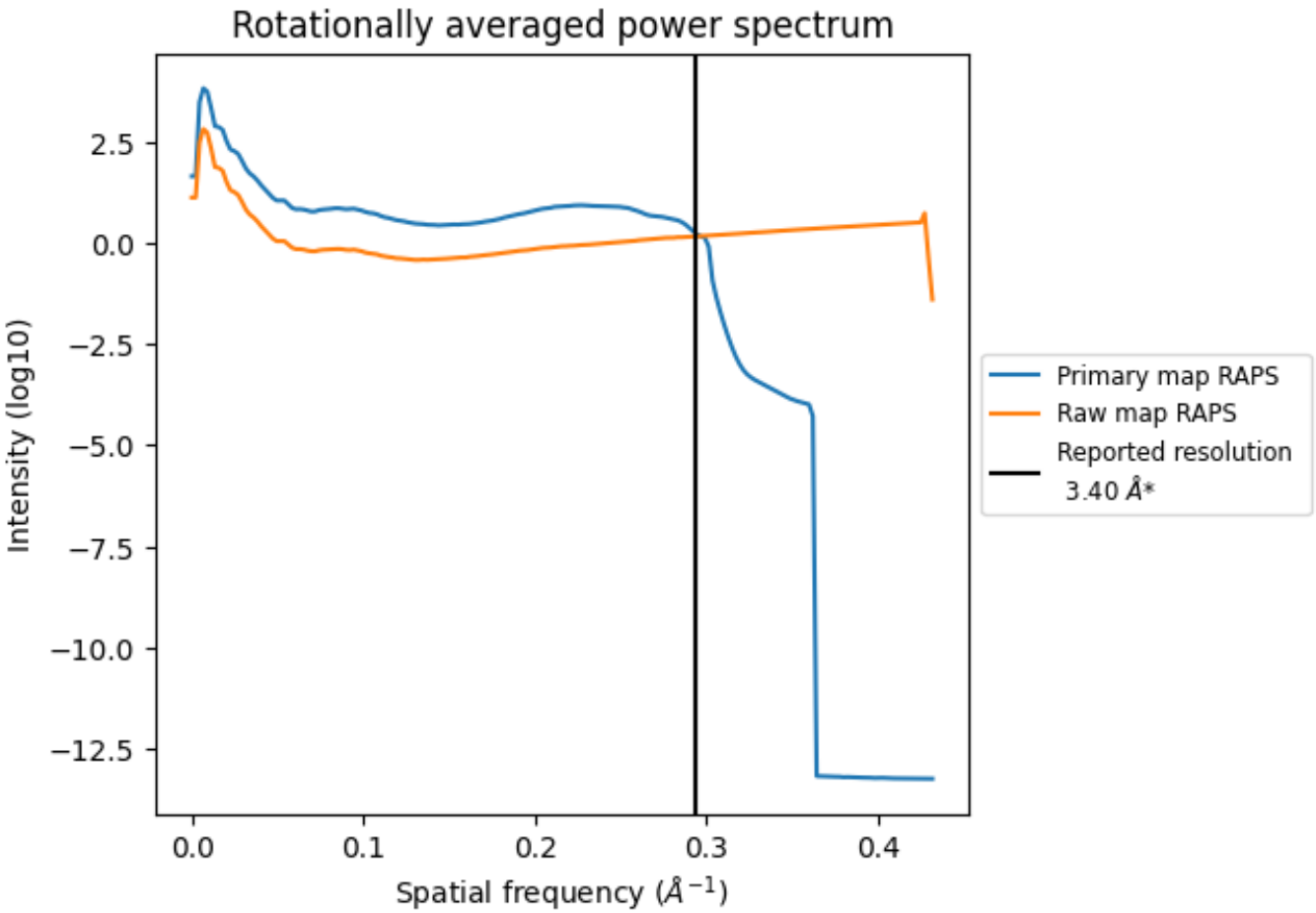
7.2 Volume estimate



The volume at the recommended contour level is 64 nm^3; this corresponds to an approximate mass of 58 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)

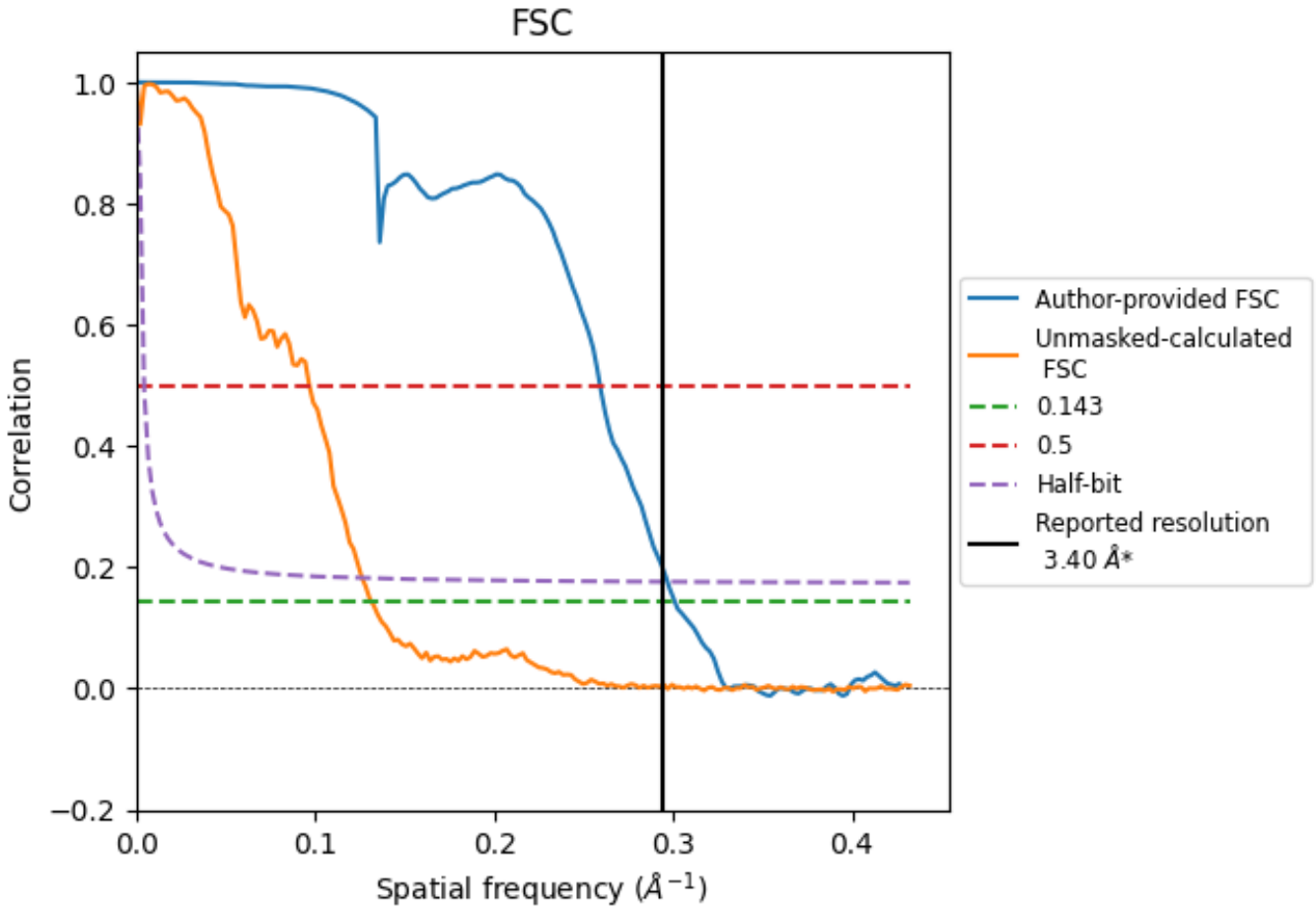


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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)

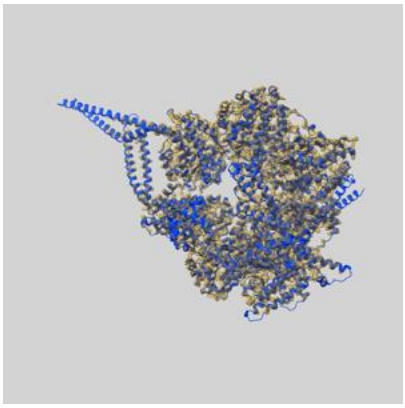
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.32	3.86	3.37
Unmasked-calculated*	7.60	10.33	7.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.60 differs from the reported value 3.4 by more than 10 %

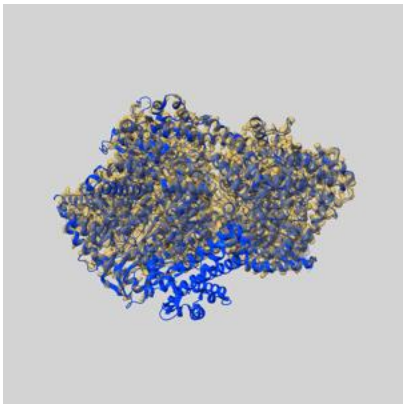
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46857 and PDB model 9DH6. Per-residue inclusion information can be found in section 3 on page 5.

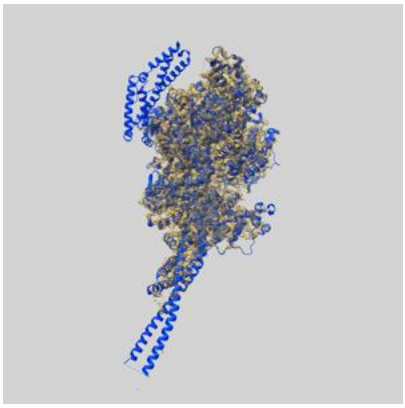
9.1 Map-model overlay



X



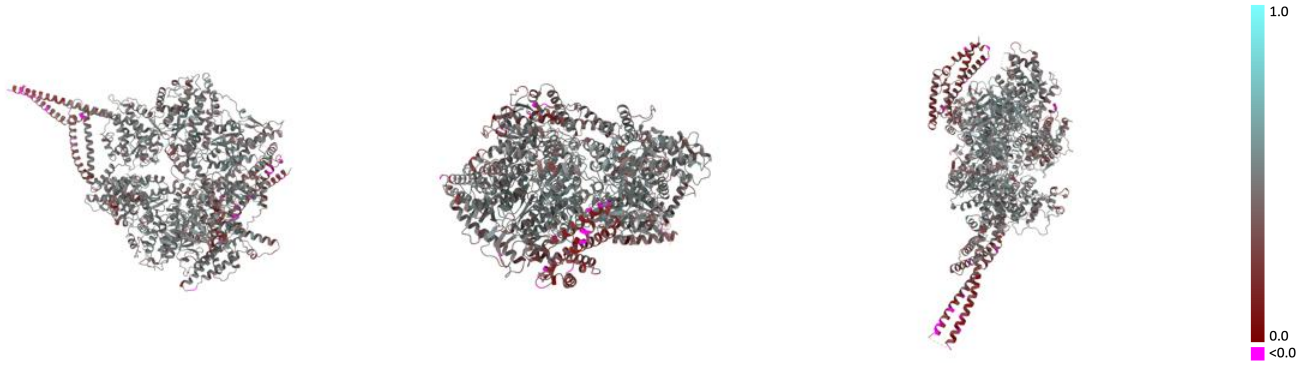
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

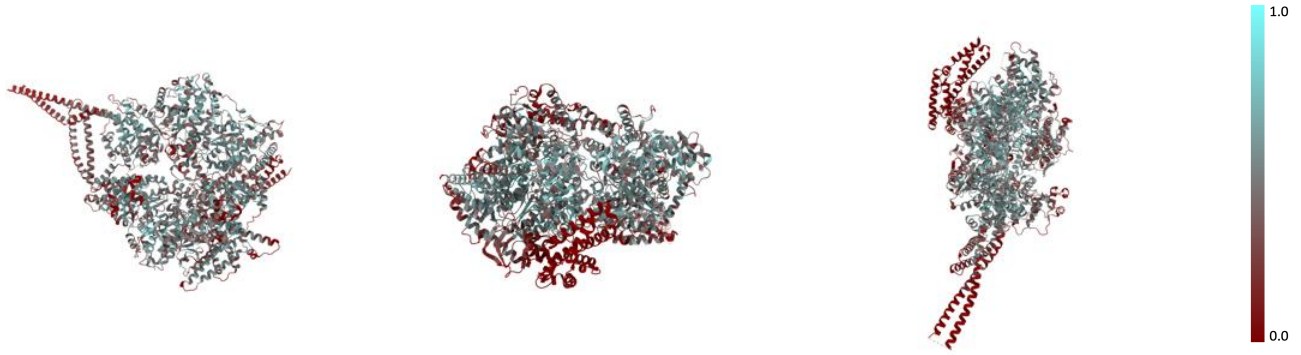
9.2 Q-score mapped to coordinate model (i)



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.

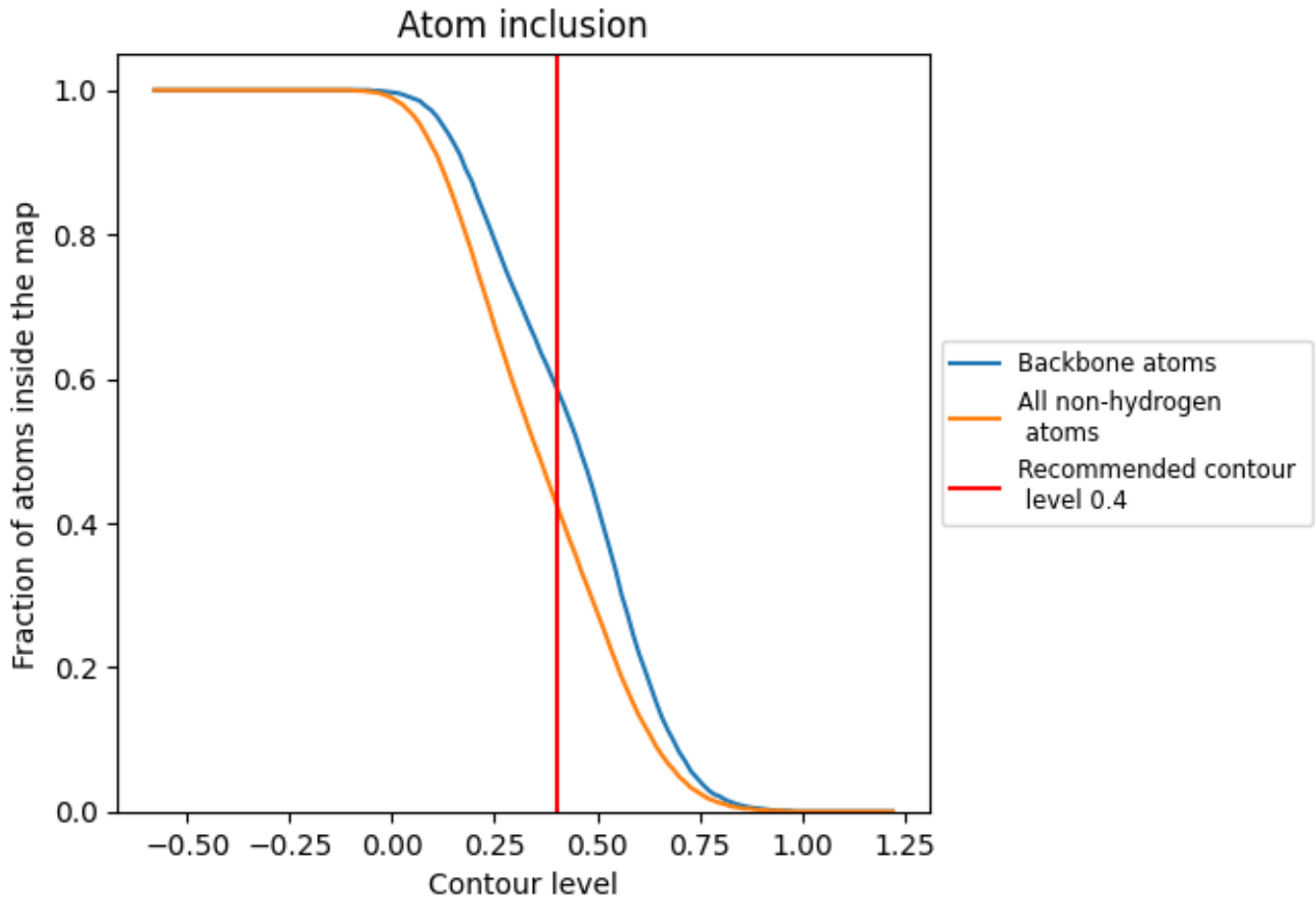
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 43% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4270	0.4420
A	0.4270	0.4420