Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 07:37 PM UTC

PDB ID	:	9BMH / pdb_00009bmh
EMDB ID	:	EMD-44699
Title	:	State-4 of motor domain from full-length human dynein-1 in 5mM ATPVi
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	2.80 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:

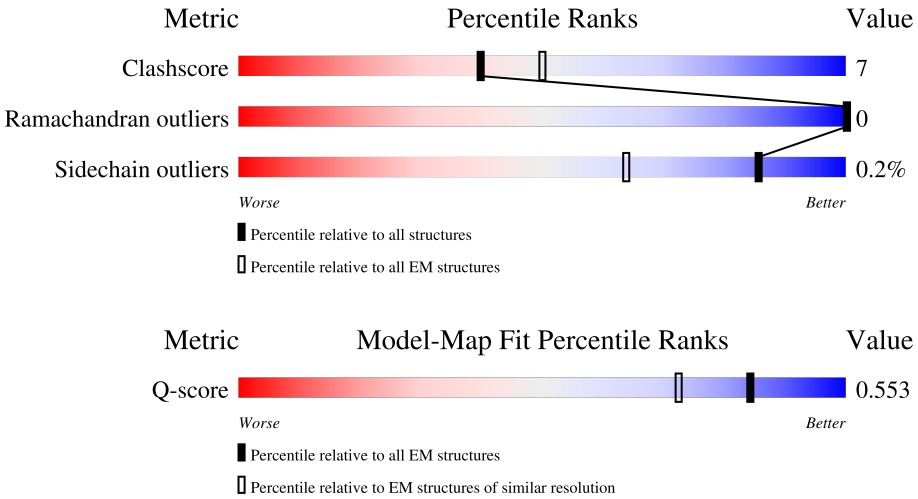
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	50% 11% 38%

2 Entry composition

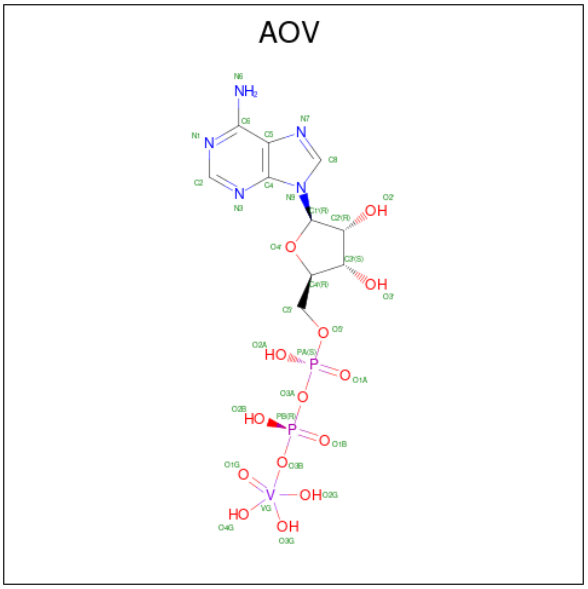
There are 5 unique types of molecules in this entry. The entry contains 23044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

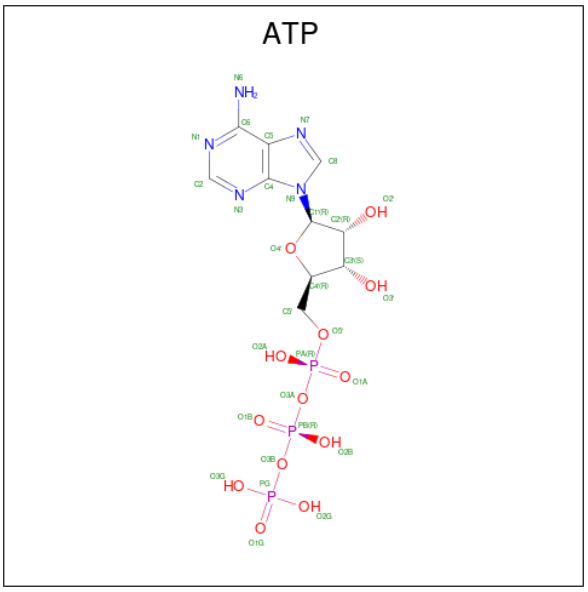
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2859	22925	14595	3960	4257	113	0	0

- Molecule 2 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$) (labeled as "Ligand of Interest" by depositor).



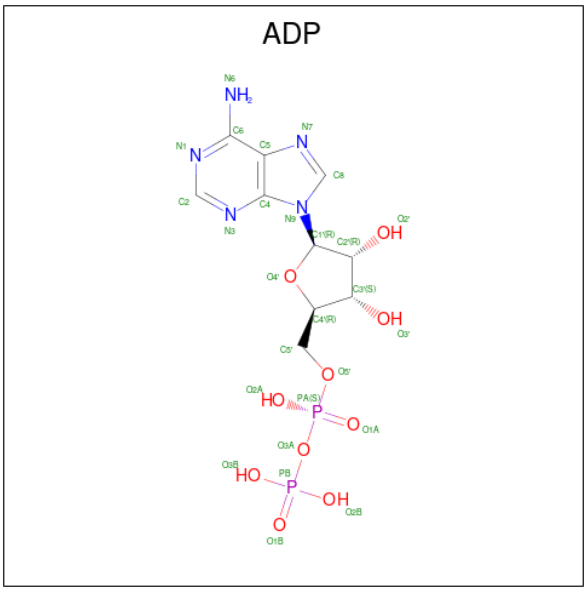
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	V	
2	A	1	32	10	5	14	2	1	0

- 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 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
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

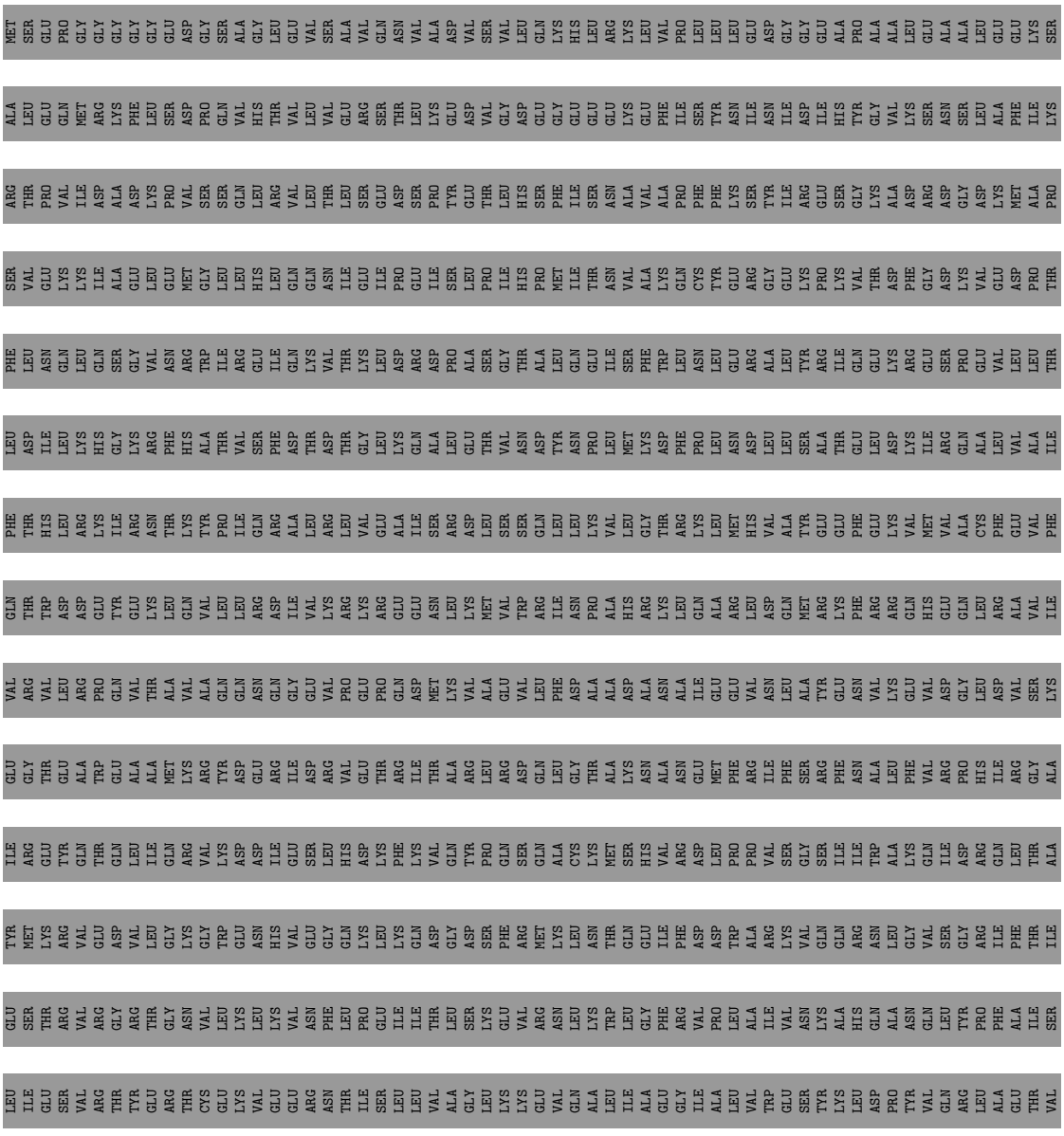
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	2	2	2	0

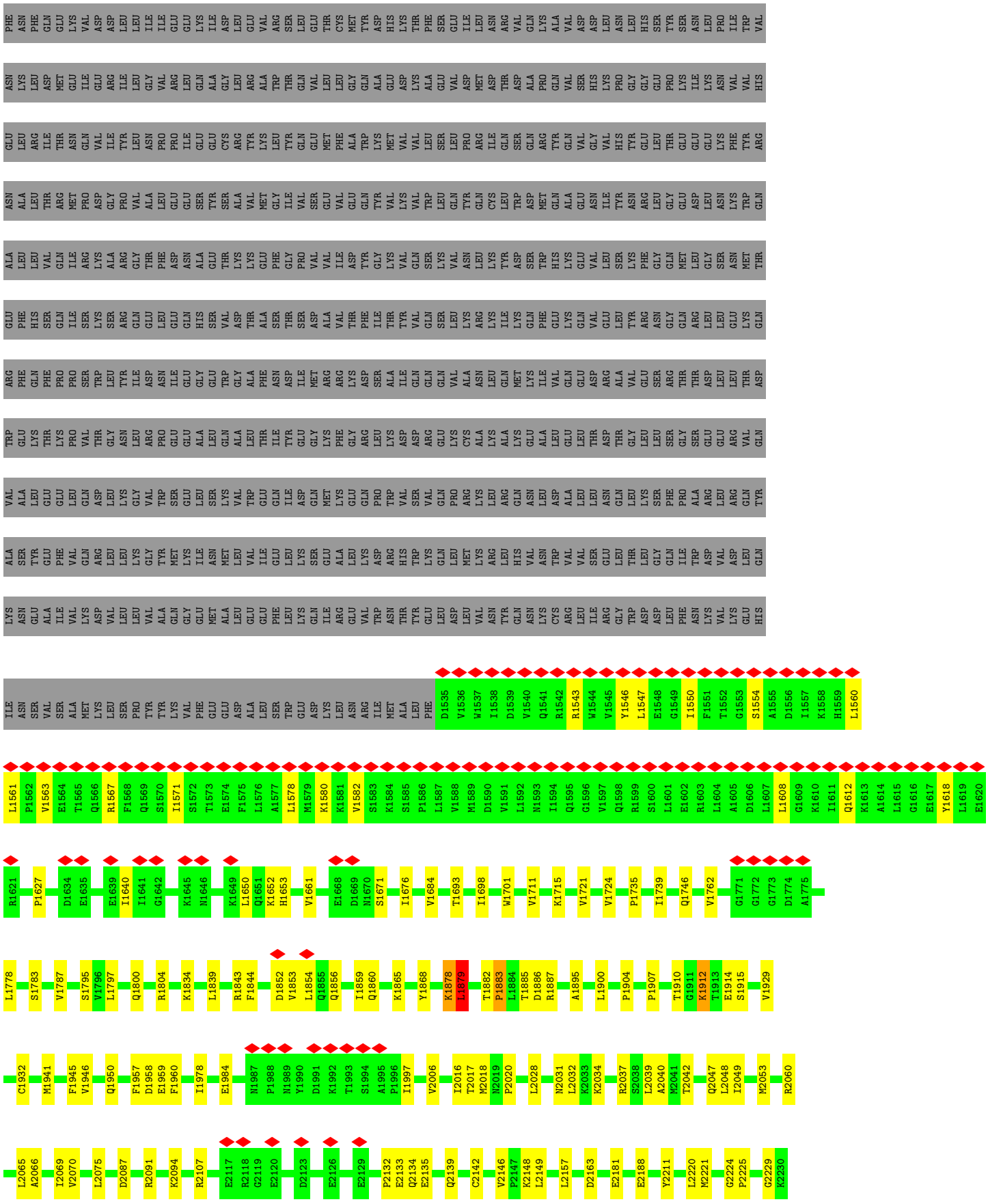
3 Residue-property plots (i)

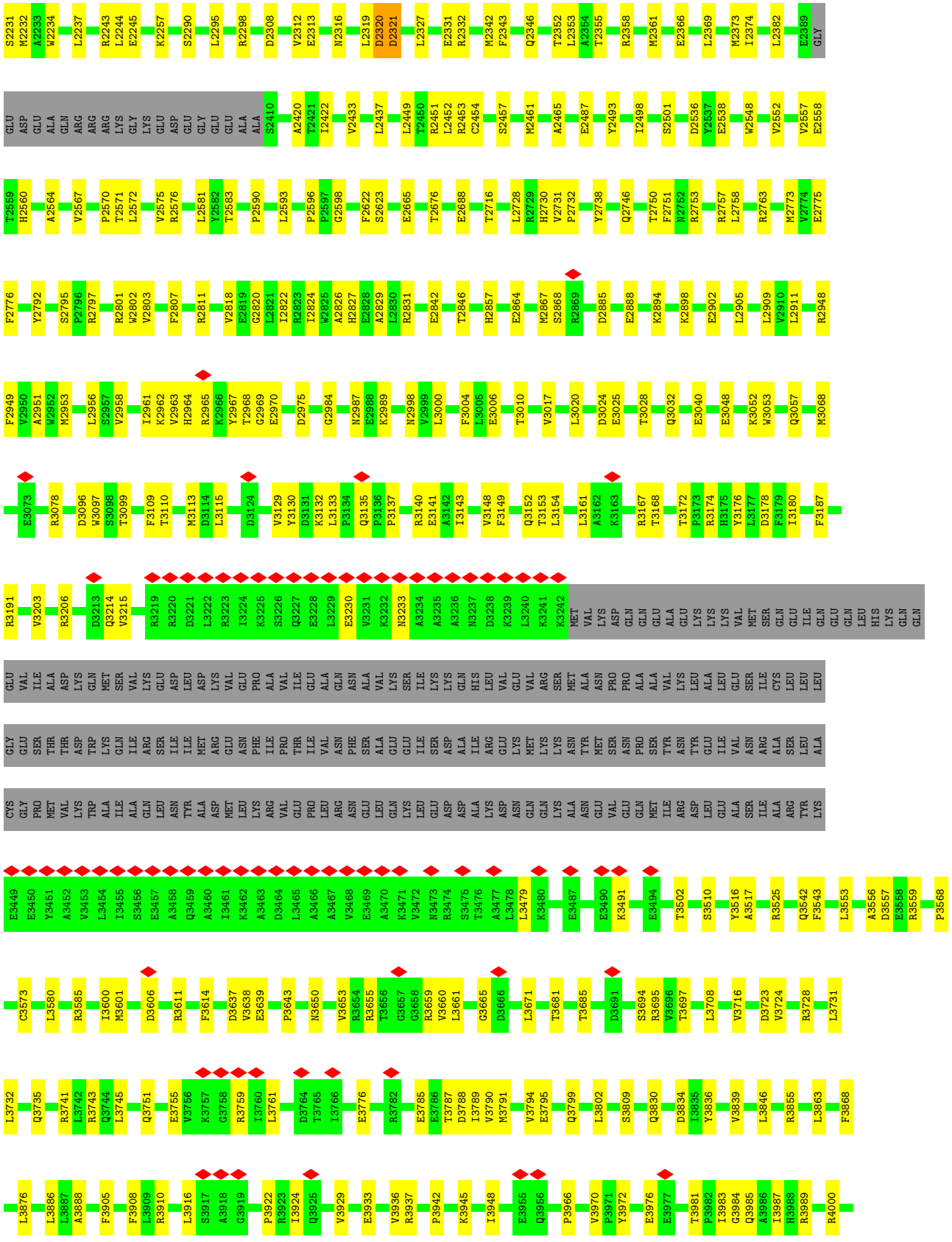
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

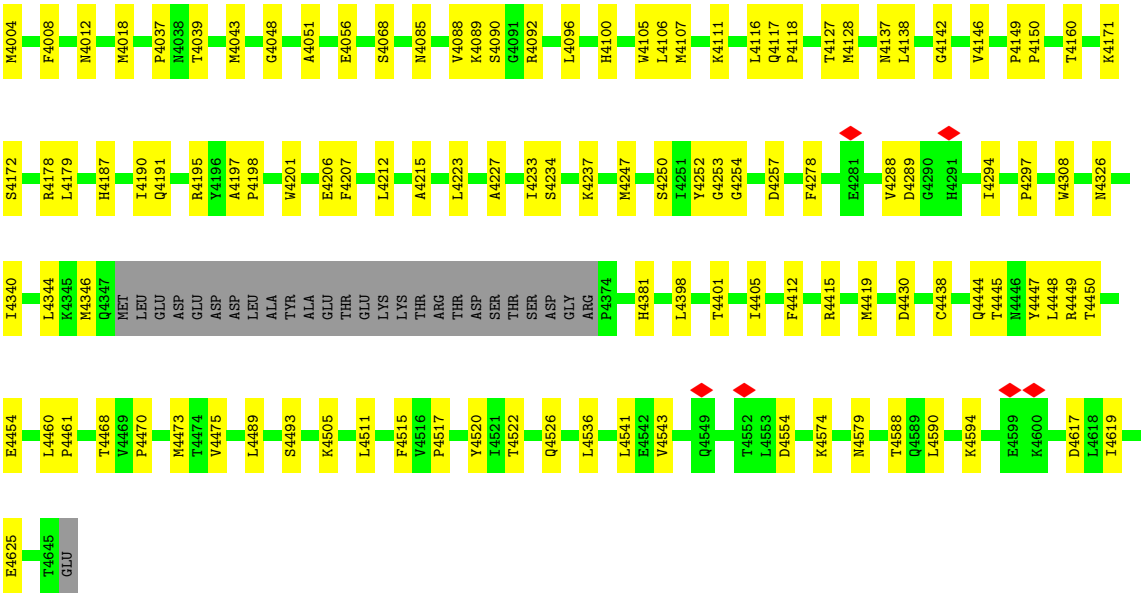
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

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 HIS
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 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 GLY GLU LEU THR GLU GLU GLU LYS PHE TYR ARG
ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER TYR SER ALA VAL MET GLY ILE VAL SER GLU VAL GLU GLN 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 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 THR SER ASP VAL ALA THR PHE ILE LYS GLN PHE GLU LYS GLN VAL GLU LEU SER LYS PHE GLU GLN VAL LEU ARG ASN GLY GLN GLU LEU GLU LEU GLU LYS
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ILE MET ARG ARG LYS ASP SER ALA ILE ASP ASN LEU GLN MET LYS ILE VAL VAL GLN GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP LEU LEU THR ASP
TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN ALA LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LYS GLU ALA LEU GLU LEU THR ASP THR GLY LEU LEU SER GLY SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU LYS GLY VAL TRP SER GLU LEU GLN SER LYS VAL TRP GLU GLN ILE ASP GLN MET LYS GLU GLN LEU ARG LYS VAL TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN ASN LEU ASP ALA LEU 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 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 ASN TYR GLN ASN LYS CYS ARG CYS LEU ILE PHE ASN LYS VAL LYS GLU HIS
ILE ASN SER VAL SER ALA MET LYS LEU SER PRO TYR TYR LYS VAL PHE GLU GLU ASP ALA LEU SER TRP GLU ASP LYS LEU ASN ARG ILE MET ALA LEU PHE D1535 V1536 W1537 I1538 D1539 V1540 Q1541 R1542 R1543 W1544 V1545 Y1546 L1547 E1548 G1549 I1550 F1551 T1552 G1553 S1554 A1555 D1556 I1557 K1558 H1559 L1560
L1561 P1562 V1563 E1564 T1565 Q1566 R1567 F1568 Q1569 S1570 I1571 S1572 T1573 E1574 F1575 L1576 A1577 L1578 M1579 K1580 K1581 V1582 S1583 K1584 S1585 P1586 L1587 V1588 M1589 D1590 V1591 L1592 N1593 I1594 Q1595 G1596 V1597 Q1598 R1599 S1600 L1601 E1602 R1603 L1604 A1605 D1606 L1607 L1608 G1609 K1610 I1611 Q1612 K1613 A1614 L1615 G1616 E1617 Y1618 L1619 E1620
R1621 P1627 D1634 E1635 E1639 I1640 I1641 G1642 K1645 N1646 K1649 L1650 Q1651 K1652 H1653 V1661 E1668 D1669 N1670 S1671 I1676 V1684 T1693 I1698 W1701 V1711 K1715 V1721 V1724 P1735 I1739 Q1746 V1762 G1771 G1772 G1773 D1774 A1775
L1778 S1783 V1787 S1795 V1796 L1797 Q1800 R1804 K1834 L1839 R1843 F1844 D1852 V1853 L1854 Q1855 Q1856 I1859 Q1860 K1865 Y1868 K1878 L1879 T1882 P1883 L1884 T1885 D1886 R1887 A1895 L1900 P1904 P1907 T1910 G1911 K1912 T1913 E1914 S1915 V1929
C1932 M1941 F1945 V1946 Q1950 F1957 D1958 E1959 F1960 I1978 E1984 N1987 P1988 N1989 Y1990 D1991 K1992 T1993 S1994 A1995 P1996 I1997 V2006 I2016 T2017 M2018 N2019 P2020 L2028 N2031 L2032 K2033 K2034 R2037 S2038 L2039 A2040 M2041 T2042 Q2047 L2048 I2049 M2053 R2060
L2065 A2066 I2069 V2070 L2075 D2087 R2091 K2094 R2107 E2117 R2118 G2119 E2120 D2123 E2126 E2129 P2132 E2133 Q2134 E2135 Q2139 C2142 V2146 P2147 K2148 L2149 L2157 D2163 E2181 E2188 Y2211 L2220 M2221 G2224 P2225 G2229 K2230




M4004 F4008 N4012 M4018 P4037 N4038 T4039 M4043 G4048 A4051 E4056 S4068 N4085 V4088 K4089 S4090 G4091 R4092 L4096 H4100 W4105 L4106 M4107 K4111 L4116 Q4117 P4118 T4127 M4128 N4137 L4138 G4142 V4146 P4149 P4150 T4160 K4171
S4172 R4178 L4179 H4187 I4190 Q4191 R4195 Y4196 A4197 P4198 W4201 E4206 F4207 L4212 A4215 L4223 A4227 I4233 S4234 K4237 M4247 S4250 I4251 Y4252 G4253 G4254 D4257 F4278 E4281 V4288 D4289 G4290 H4291 I4294 P4297 W4308 N4326
I4340 L4344 K4345 M4346 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 H4381 L4398 T4401 I4405 F4412 R4415 M4419 D4430 C4438 Q4444 T4445 N4446 Y4447 L4448 R4449 T4450
E4454 L4460 P4461 T4468 V4469 P4470 M4473 T4474 V4475 L4489 S4493 K4505 L4511 F4515 V4516 P4517 Y4520 I4521 T4522 Q4526 L4536 L4541 E4542 V4543 Q4549 T4552 L4553 D4554 K4574 N4579 T4588 Q4589 L4590 K4594 E4599 K4600 D4617 L4618 I4619
E4625 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248329	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)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.561	Depositor
Minimum map value	-1.593	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.3	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, MG, ATP, AOV

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	0.23	1/23409 (0.0%)	0.39	11/31728 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	SER	CA-CB	-5.41	1.45	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2020	PRO	N-CA-CB	-10.12	94.55	103.35
1	A	2320	ASP	CB-CA-C	-9.59	102.42	114.40
1	A	1883	PRO	N-CA-CB	-6.92	95.98	103.25
1	A	1886	ASP	N-CA-C	-6.67	104.78	113.12
1	A	1885	THR	N-CA-C	-6.60	105.19	113.18
1	A	2020	PRO	N-CA-C	6.41	121.40	111.21
1	A	2319	LEU	N-CA-CB	-6.40	101.73	110.56
1	A	1879	LEU	N-CA-CB	-6.37	100.04	110.43
1	A	1885	THR	CA-CB-OG1	-5.56	101.27	109.60
1	A	1912	LYS	N-CA-CB	-5.11	102.65	110.07
1	A	2321	ASP	N-CA-C	-5.10	106.75	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22925	0	22997	326	0
2	A	32	0	12	3	0
3	A	31	0	12	2	0
4	A	54	0	24	1	0
5	A	2	0	0	0	0
All	All	23044	0	23045	326	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 (326) 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:2753:ARG:HA	1:A:2763:ARG:HH22	1.30	0.95
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.66	0.77
1:A:3799:GLN:HA	1:A:3802:LEU:HD23	1.66	0.76
1:A:2688:GLU:OE1	1:A:2730:HIS:NE2	2.18	0.75
1:A:3639:GLU:OE2	1:A:4111:LYS:NZ	2.16	0.71
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.73	0.70
1:A:1797:LEU:HD11	1:A:2060:ARG:HH21	1.56	0.69
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.73	0.69
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.76	0.68
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.76	0.68
1:A:4470:PRO:HD2	1:A:4473:MET:HE3	1.75	0.68
1:A:3113:MET:HE2	1:A:3115:LEU:HD21	1.75	0.67
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.76	0.67
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.28	0.67
1:A:3972:TYR:OH	1:A:3976:GLU:OE1	2.13	0.66
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.77	0.66
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.79	0.65
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.27	0.65
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.28	0.65
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.78	0.65
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.61	0.65
1:A:1984:GLU:HG3	1:A:1997:ILE:HD12	1.79	0.64
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.80	0.64
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.79	0.64
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.30	0.63
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3735:GLN:NE2	1:A:3788:ASP:OD1	2.29	0.62
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.81	0.62
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.33	0.62
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.33	0.62
1:A:1543:ARG:HA	1:A:1546:TYR:CE1	2.34	0.61
1:A:3068:MET:HE1	1:A:3078:ARG:HG3	1.82	0.61
1:A:1907:PRO:HD3	1:A:2042:THR:HG22	1.83	0.61
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.84	0.60
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.35	0.59
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.15	0.59
1:A:4574:LYS:NZ	1:A:4625:GLU:OE2	2.32	0.59
1:A:1640:ILE:HG23	1:A:1650:LEU:HD21	1.83	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.85	0.58
1:A:3109:PHE:HD2	1:A:3180:ILE:HG22	1.67	0.58
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.37	0.58
1:A:1932:CYS:HB2	1:A:1959:GLU:O	2.04	0.58
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.38	0.57
1:A:2320:ASP:OD1	1:A:2358:ARG:NE	2.37	0.57
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.85	0.57
1:A:3886:LEU:HD12	1:A:4346:MET:HE3	1.86	0.57
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.23	0.57
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.86	0.57
1:A:1563:VAL:HG22	1:A:1567:ARG:HE	1.68	0.56
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.23	0.56
1:A:3745:LEU:HD11	1:A:3776:GLU:HG3	1.87	0.56
1:A:1900:LEU:HD11	1:A:2037:ARG:HG2	1.86	0.56
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	1.88	0.56
1:A:1546:TYR:OH	1:A:1612:GLN:OE1	2.21	0.56
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.54	0.56
1:A:4288:VAL:HG11	1:A:4294:ILE:HG12	1.88	0.56
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.88	0.56
1:A:2220:LEU:HD12	1:A:2342:MET:HG2	1.88	0.56
1:A:2557:VAL:HG23	1:A:2750:THR:HG22	1.88	0.56
1:A:3728:ARG:HB2	1:A:3794:VAL:HG11	1.87	0.56
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.88	0.55
1:A:2894:LYS:HG3	1:A:2911:LEU:HD12	1.88	0.55
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.39	0.55
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.39	0.55
1:A:3028:THR:O	1:A:3032:GLN:HG3	2.07	0.55
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.87	0.55
1:A:2949:PHE:CZ	1:A:2953:MET:HE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2037:ARG:HH21	1:A:4250:SER:HB3	1.72	0.55
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.34	0.54
1:A:4191:GLN:NE2	1:A:4207:PHE:O	2.36	0.54
1:A:2369:LEU:HD12	1:A:2373:MET:HE2	1.88	0.54
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.40	0.54
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.89	0.54
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.72	0.54
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.07	0.54
1:A:2558:GLU:OE1	1:A:2560:HIS:NE2	2.41	0.54
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.40	0.54
1:A:1735:PRO:O	1:A:1739:ILE:HG12	2.07	0.54
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.72	0.54
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.89	0.53
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	1.89	0.53
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.36	0.53
1:A:3989:ARG:HB2	1:A:4004:MET:HE2	1.89	0.53
1:A:4450:THR:O	1:A:4454:GLU:HG3	2.07	0.53
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.90	0.53
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.91	0.53
1:A:1795:SER:O	1:A:1800:GLN:NE2	2.34	0.53
1:A:2353:LEU:HG	1:A:2353:LEU:O	2.07	0.53
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.91	0.52
1:A:1853:VAL:HG13	1:A:1854:LEU:HD22	1.90	0.52
1:A:2826:ALA:HB2	1:A:2867:MET:HE1	1.91	0.52
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.91	0.52
1:A:2225:PRO:HB2	1:A:2366:GLU:HG3	1.91	0.52
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.91	0.52
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.36	0.52
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.91	0.52
1:A:1684:VAL:HG12	1:A:1746:GLN:NE2	2.25	0.52
1:A:4171:LYS:HG2	1:A:4172:SER:H	1.74	0.52
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.45	0.51
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.51
1:A:1941:MET:HE2	1:A:1960:PHE:HE1	1.76	0.51
1:A:2075:LEU:HD22	1:A:4522:THR:HG23	1.92	0.51
1:A:2964:HIS:HA	1:A:3643:PRO:HD2	1.93	0.51
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.91	0.51
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.44	0.51
1:A:4489:LEU:HD11	1:A:4515:PHE:HE1	1.74	0.51
1:A:2753:ARG:HA	1:A:2763:ARG:NH2	2.13	0.51
1:A:3109:PHE:CD2	1:A:3180:ILE:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.92	0.51
1:A:2313:GLU:OE2	1:A:2352:THR:OG1	2.29	0.51
1:A:2885:ASP:HB3	1:A:2888:GLU:OE1	2.10	0.51
1:A:4107:MET:O	1:A:4111:LYS:HG2	2.11	0.51
1:A:3795:GLU:O	1:A:3799:GLN:HG2	2.10	0.51
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.43	0.51
1:A:3985:GLN:O	1:A:3989:ARG:HG3	2.11	0.51
1:A:2221:MET:SD	1:A:2361:MET:HE1	2.51	0.50
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.47	0.50
1:A:3187:PHE:CE2	1:A:3191:ARG:HD2	2.47	0.50
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.11	0.50
1:A:2963:VAL:HG13	1:A:3000:LEU:HD11	1.93	0.50
1:A:3759:ARG:HH21	1:A:3761:LEU:HB2	1.77	0.50
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.94	0.50
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.27	0.50
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.93	0.50
1:A:2564:ALA:HB3	1:A:2567:VAL:CG2	2.41	0.49
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.94	0.49
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.94	0.49
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.78	0.49
1:A:1550:ILE:O	1:A:1554:SER:OG	2.30	0.49
1:A:1914:GLU:HG3	2:A:4701:AOV:H2'	1.93	0.49
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.95	0.49
1:A:3650:ASN:HD21	1:A:3695:ARG:NH1	2.09	0.49
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.93	0.49
1:A:1543:ARG:HB3	1:A:1608:LEU:HD12	1.94	0.49
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.94	0.49
1:A:2827:HIS:CE1	1:A:2831:ARG:HH11	2.31	0.48
1:A:4090:SER:OG	1:A:4092:ARG:HG3	2.13	0.48
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	1.96	0.48
1:A:3728:ARG:O	1:A:3732:LEU:HG	2.14	0.48
1:A:2572:LEU:O	1:A:2575:VAL:HG22	2.13	0.48
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.95	0.48
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.95	0.48
1:A:4526:GLN:HA	1:A:4536:LEU:HD21	1.95	0.48
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.94	0.48
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.48	0.48
1:A:2792:TYR:OH	1:A:2842:GLU:OE1	2.29	0.48
1:A:1907:PRO:HG2	1:A:1910:THR:HG21	1.95	0.48
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.95	0.48
1:A:3732:LEU:HD23	1:A:3791:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2229:GLY:HA2	3:A:4702:ATP:O2A	2.14	0.47
1:A:2091:ARG:NH1	2:A:4701:AOV:O1G	2.38	0.47
1:A:3006:GLU:O	1:A:3010:THR:HG23	2.15	0.47
1:A:3149:PHE:O	1:A:3153:THR:HG23	2.14	0.47
1:A:4117:GLN:HG2	1:A:4117:GLN:O	2.13	0.47
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.14	0.47
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.49	0.47
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.50	0.47
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.14	0.47
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.97	0.47
1:A:3886:LEU:CD1	1:A:4346:MET:HE3	2.45	0.47
1:A:2075:LEU:HD13	1:A:4536:LEU:HD13	1.97	0.47
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.40	0.47
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.97	0.46
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.97	0.46
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.15	0.46
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.97	0.46
1:A:4043:MET:HE3	1:A:4051:ALA:HB1	1.98	0.46
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.98	0.46
1:A:3735:GLN:NE2	1:A:3787:THR:HG23	2.30	0.46
1:A:1578:LEU:O	1:A:1582:VAL:HG12	2.15	0.46
1:A:1711:VAL:O	1:A:1715:LYS:HG2	2.16	0.46
1:A:2028:LEU:HG	1:A:2032:LEU:HD23	1.98	0.46
1:A:2571:THR:HG22	1:A:2746:GLN:NE2	2.31	0.46
1:A:2948:ARG:HG2	1:A:2958:VAL:HG11	1.97	0.46
1:A:2188:GLU:OE2	1:A:2243:ARG:NH2	2.48	0.46
1:A:4197:ALA:HB3	1:A:4198:PRO:HD3	1.98	0.46
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.48	0.46
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.49	0.46
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.98	0.46
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.98	0.46
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.81	0.46
1:A:1800:GLN:OE1	1:A:1804:ARG:NE	2.49	0.45
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.80	0.45
1:A:3846:LEU:HD22	1:A:3855:ARG:HG2	1.98	0.45
1:A:1844:PHE:HE1	1:A:1859:ILE:HG23	1.81	0.45
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	1.97	0.45
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.51	0.45
1:A:3048:GLU:O	1:A:3052:LYS:HG2	2.16	0.45
1:A:2018:MET:HB2	1:A:2018:MET:HE3	1.44	0.45
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3167:ARG:NH1	1:A:3685:THR:HA	2.32	0.45
1:A:3653:VAL:HG11	1:A:3671:LEU:HD22	1.98	0.45
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.97	0.45
1:A:1661:VAL:HG13	1:A:1676:ILE:HB	1.98	0.45
1:A:1929:VAL:H	1:A:2332:ARG:HH22	1.64	0.45
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.51	0.45
1:A:3741:ARG:HA	1:A:3741:ARG:HD2	1.65	0.45
1:A:4085:ASN:O	1:A:4089:LYS:NZ	2.37	0.45
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.98	0.45
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.49	0.45
1:A:2572:LEU:O	1:A:2576:ARG:HG3	2.16	0.45
1:A:3230:GLU:HA	1:A:3233:ASN:HD21	1.81	0.45
1:A:2320:ASP:HB3	1:A:2321:ASP:H	1.40	0.45
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.99	0.45
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.17	0.45
1:A:3948:ILE:HD12	1:A:3948:ILE:H	1.82	0.45
1:A:4178:ARG:HD3	1:A:4278:PHE:CD2	2.52	0.45
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.82	0.44
1:A:2962:LYS:HG3	1:A:3665:GLY:HA2	1.98	0.44
1:A:3601:MET:CE	1:A:3611:ARG:HB2	2.47	0.44
1:A:4468:THR:HG21	1:A:4617:ASP:OD1	2.16	0.44
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.98	0.44
1:A:3024:ASP:O	1:A:3028:THR:HG23	2.17	0.44
1:A:1652:LYS:HG3	1:A:1653:HIS:CD2	2.52	0.44
1:A:1852:ASP:O	1:A:1856:GLN:NE2	2.50	0.44
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.99	0.44
1:A:1878:LYS:HB3	1:A:1878:LYS:HE3	1.41	0.44
1:A:2797:ARG:O	1:A:2801:ARG:HG3	2.18	0.44
1:A:2909:LEU:HA	4:A:4704:ADP:C2	2.51	0.44
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.52	0.44
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.18	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.52	0.43
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.00	0.43
1:A:2457:SER:HB2	1:A:2501:SER:HB3	2.00	0.43
1:A:3203:VAL:O	1:A:3206:ARG:HG2	2.18	0.43
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.89	0.43
1:A:1560:LEU:O	1:A:1561:LEU:HD23	2.19	0.43
1:A:1929:VAL:HG13	1:A:1958:ASP:OD2	2.19	0.43
1:A:3161:LEU:HB2	1:A:3168:THR:HG22	2.01	0.43
1:A:2820:GLY:O	1:A:2824:ILE:HG13	2.18	0.43
1:A:1561:LEU:HD21	1:A:1618:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.84	0.43
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.19	0.43
1:A:3751:GLN:O	1:A:3755:GLU:HG2	2.17	0.43
1:A:4594:LYS:HE3	1:A:4594:LYS:HB3	1.93	0.43
1:A:1834:LYS:HD3	1:A:1834:LYS:HA	1.78	0.43
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.51	0.43
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.83	0.43
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.54	0.43
1:A:3922:PRO:HD2	1:A:3936:VAL:HG11	2.00	0.43
1:A:2905:LEU:HD21	1:A:2948:ARG:CZ	2.49	0.43
1:A:3024:ASP:OD1	1:A:3025:GLU:N	2.52	0.43
1:A:4043:MET:HB2	1:A:4127:THR:HG22	1.99	0.43
1:A:4048:GLY:HA3	1:A:4206:GLU:OE1	2.19	0.43
1:A:3214:GLN:HG3	1:A:3759:ARG:CZ	2.49	0.42
1:A:1547:LEU:HD23	1:A:1547:LEU:HA	1.81	0.42
1:A:3910:ARG:NH1	1:A:4344:LEU:HD11	2.34	0.42
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.54	0.42
1:A:3491:LYS:HA	1:A:3491:LYS:HD3	1.77	0.42
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	2.01	0.42
1:A:2552:VAL:HG22	1:A:2575:VAL:HG11	2.02	0.42
1:A:3215:VAL:HG21	1:A:3479:LEU:HD11	2.00	0.42
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.96	0.42
1:A:4448:LEU:HD23	1:A:4448:LEU:HA	1.91	0.42
1:A:2163:ASP:OD2	1:A:4526:GLN:HG3	2.20	0.42
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.19	0.42
1:A:1739:ILE:HG23	1:A:1804:ARG:HD2	2.02	0.42
1:A:1945:PHE:HB3	1:A:1978:ILE:HD11	2.01	0.42
1:A:3614:PHE:HD2	1:A:3637:ASP:O	2.02	0.42
1:A:3983:ILE:O	1:A:3987:ILE:HG13	2.19	0.42
1:A:1783:SER:O	1:A:1787:VAL:HG13	2.20	0.42
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.02	0.42
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.60	0.42
1:A:2758:LEU:HD11	1:A:2807:PHE:CE1	2.54	0.42
1:A:2949:PHE:CE2	1:A:2953:MET:HE3	2.54	0.42
1:A:3868:PHE:CZ	1:A:4018:MET:HG2	2.55	0.42
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.52	0.42
1:A:2040:ALA:HB1	1:A:4257:ASP:HB3	2.02	0.42
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	2.02	0.42
1:A:2968:THR:HG23	1:A:2970:GLU:HG2	2.00	0.42
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	2.02	0.42
1:A:2622:PHE:HB2	1:A:2665:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:LEU:HD11	1:A:2060:ARG:NH2	2.31	0.41
1:A:3886:LEU:HD23	1:A:3886:LEU:HA	1.89	0.41
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	2.02	0.41
1:A:2031:ASN:HA	1:A:2034:LYS:HE3	2.01	0.41
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	2.02	0.41
1:A:2221:MET:CG	1:A:2343:PHE:HB2	2.49	0.41
1:A:4444:GLN:HG2	1:A:4449:ARG:HG3	2.02	0.41
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	2.02	0.41
1:A:3659:ARG:HE	1:A:3661:LEU:HD21	1.85	0.41
1:A:4056:GLU:OE1	1:A:4068:SER:OG	2.31	0.41
1:A:2716:THR:HB	1:A:4445:THR:HB	2.02	0.41
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	2.01	0.41
1:A:3556:ALA:HB3	1:A:3743:ARG:NH1	2.36	0.41
1:A:3908:PHE:CZ	1:A:4340:ILE:HD11	2.55	0.41
1:A:3929:VAL:HG12	1:A:3933:GLU:OE2	2.20	0.41
1:A:4415:ARG:HG2	1:A:4419:MET:HE2	2.03	0.41
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	2.01	0.41
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.86	0.41
1:A:4215:ALA:HB1	1:A:4247:MET:HE2	2.02	0.41
1:A:4288:VAL:HG23	1:A:4289:ASP:OD1	2.21	0.41
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	2.02	0.41
1:A:2864:GLU:O	1:A:2868:SER:OG	2.31	0.41
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	2.03	0.41
1:A:2049:ILE:O	1:A:2053:MET:HG3	2.21	0.41
1:A:2965:ARG:NH1	1:A:3614:PHE:O	2.48	0.41
1:A:3230:GLU:HA	1:A:3233:ASN:ND2	2.35	0.41
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.61	0.41
1:A:3942:PRO:HA	1:A:3945:LYS:HG3	2.02	0.41
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.54	0.41
1:A:3728:ARG:NH1	1:A:3732:LEU:HD11	2.36	0.41
1:A:4039:THR:HG23	1:A:4142:GLY:HA2	2.03	0.41
1:A:1571:ILE:HD13	1:A:1608:LEU:HD22	2.03	0.41
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	2.03	0.41
1:A:2758:LEU:HD13	1:A:2811:ARG:HA	2.03	0.41
1:A:2898:LYS:O	1:A:2902:GLU:HG3	2.21	0.41
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.46	0.41
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.21	0.40
1:A:3556:ALA:HA	1:A:3559:ARG:HB2	2.02	0.40
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	2.02	0.40
1:A:2984:GLY:HA2	1:A:3057:GLN:HB3	2.04	0.40
1:A:1912:LYS:NZ	2:A:4701:AOV:O4G	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2570:PRO:O	1:A:2746:GLN:NE2	2.54	0.40
1:A:3502:THR:HB	1:A:3543:PHE:HA	2.04	0.40
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.22	0.40
1:A:1762:VAL:HG13	1:A:1778:LEU:HD11	2.04	0.40
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	2.03	0.40
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.21	0.40
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	2.02	0.40
1:A:3905:PHE:HZ	1:A:4008:PHE:CZ	2.40	0.40
1:A:4398:LEU:HD21	1:A:4493:SER:HA	2.03	0.40
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.93	0.40
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	2.02	0.40
1:A:1580:LYS:HD3	1:A:1580:LYS:HA	1.91	0.40
1:A:2773:MET:HE2	1:A:2773:MET:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2851/4646 (61%)	2803 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2532/4125 (61%)	2527 (100%)	5 (0%)	87 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1878	LYS
1	A	1879	LEU
1	A	1883	PRO
1	A	2094	LYS
1	A	2355	THR

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	1598	GLN
1	A	1779	HIS
1	A	1817	HIS
1	A	1855	GLN
1	A	1894	GLN
1	A	1922	GLN
1	A	2051	GLN
1	A	2079	GLN
1	A	2263	HIS
1	A	2439	HIS
1	A	2637	HIS
1	A	2698	GLN
1	A	2827	HIS
1	A	2860	ASN
1	A	2918	HIS
1	A	2954	ASN
1	A	2960	GLN
1	A	3063	HIS
1	A	3523	GLN
1	A	3563	GLN
1	A	3744	GLN
1	A	3799	GLN
1	A	3820	GLN
1	A	3877	HIS
1	A	4029	HIS
1	A	4098	ASN
1	A	4114	HIS
1	A	4295	GLN

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Mol	Chain	Res	Type
1	A	4326	ASN
1	A	4429	GLN
1	A	4490	GLN
1	A	4508	HIS
1	A	4530	GLN
1	A	4566	GLN
1	A	4579	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 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	AOV	A	4701	5	32,34,34	4.97	7 (21%)	42,56,56	2.36	12 (28%)
3	ATP	A	4702	5	32,33,33	0.74	0	48,52,52	0.64	0
4	ADP	A	4703	-	28,29,29	0.47	0	43,45,45	0.48	0
4	ADP	A	4704	-	28,29,29	0.48	0	43,45,45	0.49	0

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	AOV	A	4701	5	-	2/16/39/39	0/3/3/3
3	ATP	A	4702	5	-	6/22/38/38	0/3/3/3
4	ADP	A	4703	-	-	1/16/32/32	0/3/3/3
4	ADP	A	4704	-	-	0/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	AOV	O1G-VG	26.61	2.08	1.61
2	A	4701	AOV	C5-C4	3.59	1.45	1.39
2	A	4701	AOV	PA-O3A	-3.53	1.55	1.59
2	A	4701	AOV	C8-N9	-3.45	1.31	1.37
2	A	4701	AOV	C5-N7	-2.98	1.33	1.39
2	A	4701	AOV	C5-C6	2.39	1.47	1.41
2	A	4701	AOV	C4-N9	-2.10	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	AOV	C5-C4-N3	-7.20	116.80	126.72
2	A	4701	AOV	N3-C4-N9	5.31	136.19	127.17
2	A	4701	AOV	C4-C5-N7	-5.00	104.86	110.58
2	A	4701	AOV	C2-N3-C4	4.54	122.91	111.83
2	A	4701	AOV	N3-C2-N1	-4.07	122.42	128.58
2	A	4701	AOV	C5-N7-C8	3.59	109.09	103.45
2	A	4701	AOV	O2B-PB-O3A	3.57	116.94	107.27
2	A	4701	AOV	C2'-C1'-N9	-3.15	105.47	113.30
2	A	4701	AOV	C4-N9-C8	2.99	108.88	105.74
2	A	4701	AOV	C6-C5-N7	2.83	137.54	132.09
2	A	4701	AOV	N9-C8-N7	-2.67	110.15	113.94
2	A	4701	AOV	O3A-PB-O1B	-2.31	103.75	110.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	4701	AOV	PA-O3A-PB-O2B
3	A	4702	ATP	PA-O3A-PB-O2B
2	A	4701	AOV	PA-O3A-PB-O1B
3	A	4702	ATP	PG-O3B-PB-O2B
4	A	4703	ADP	C2'-C1'-N9-C8
3	A	4702	ATP	PG-O3B-PB-O1B
3	A	4702	ATP	PA-O3A-PB-O1B

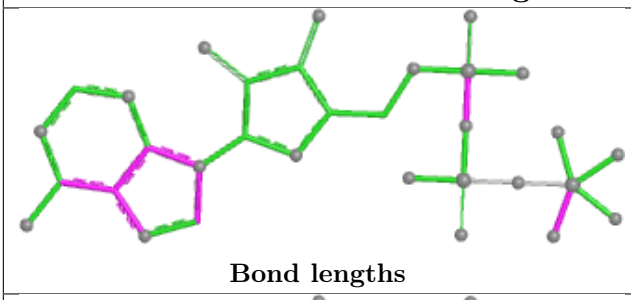
There are no ring outliers.

3 monomers are involved in 6 short contacts:

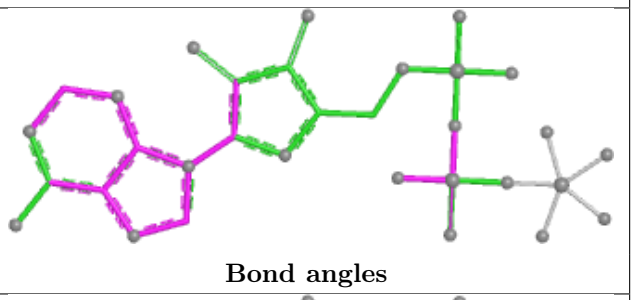
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	AOV	3	0
3	A	4702	ATP	2	0
4	A	4704	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

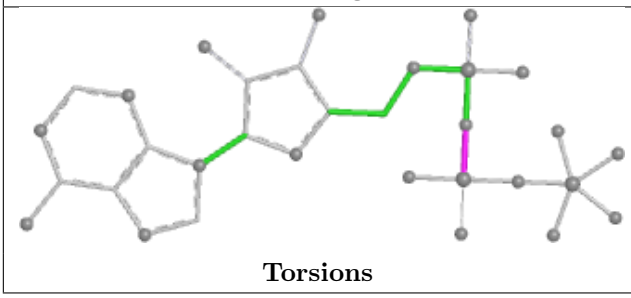
Ligand AOV A 4701



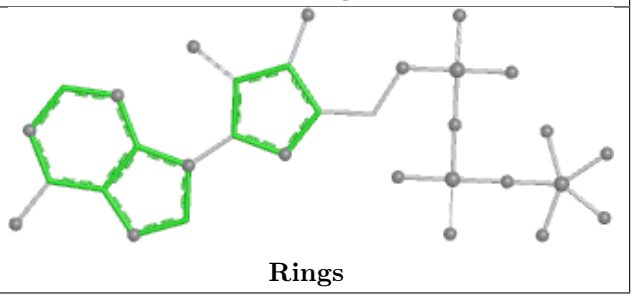
Bond lengths



Bond angles

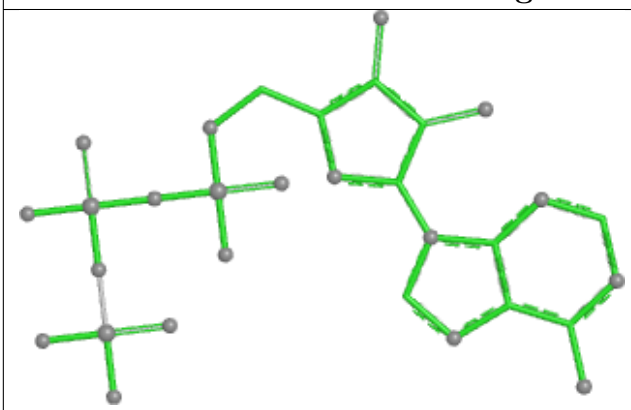


Torsions

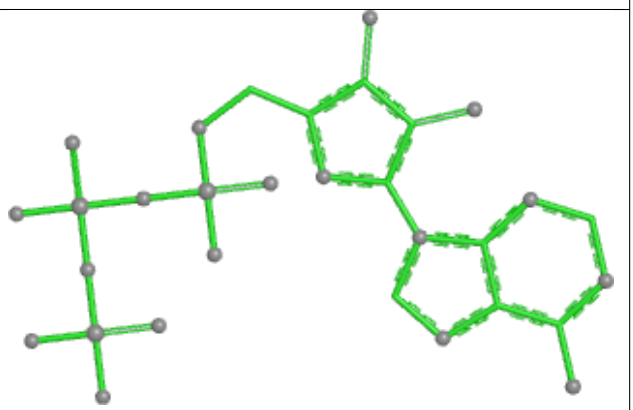


Rings

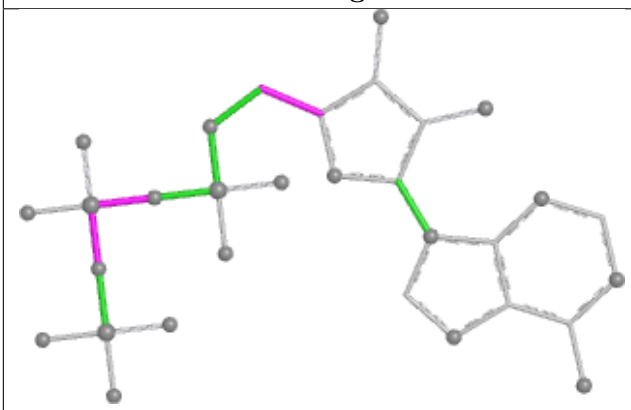
Ligand ATP A 4702



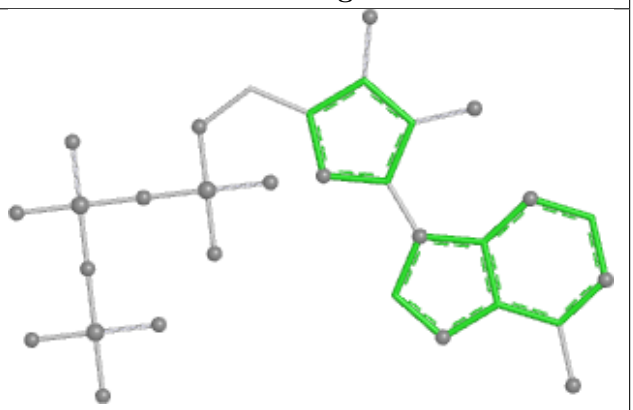
Bond lengths



Bond angles

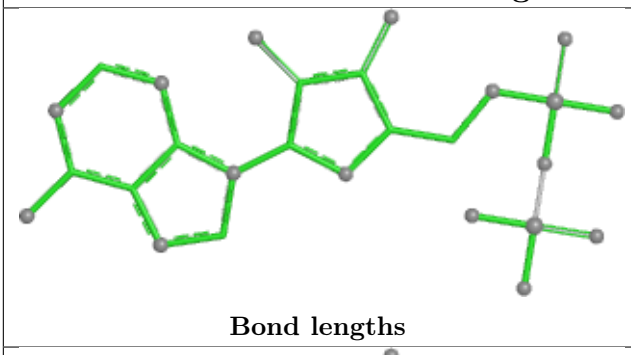


Torsions

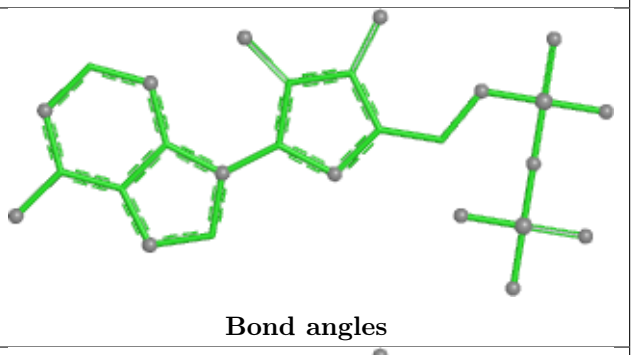


Rings

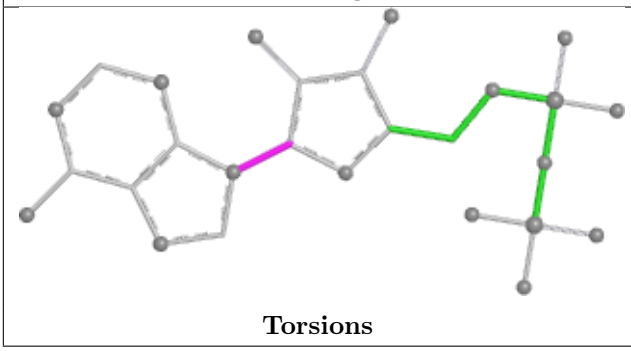
Ligand ADP A 4703



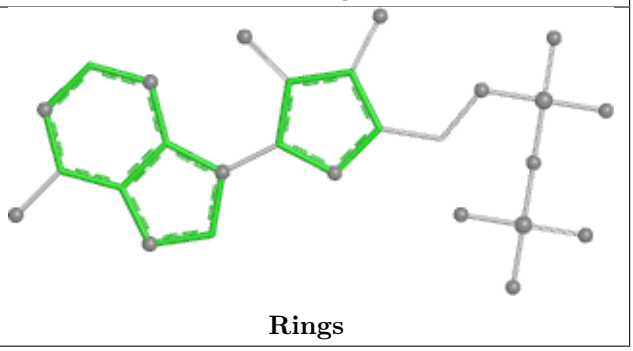
Bond lengths



Bond angles

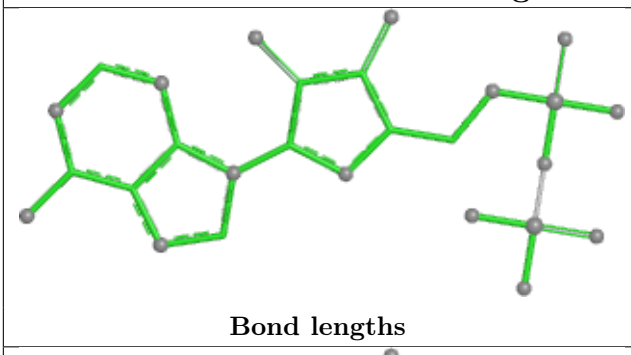


Torsions

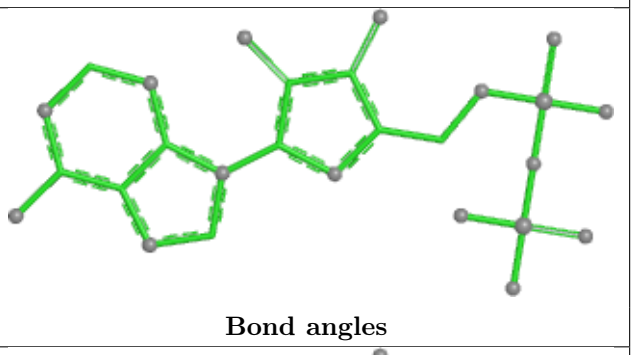


Rings

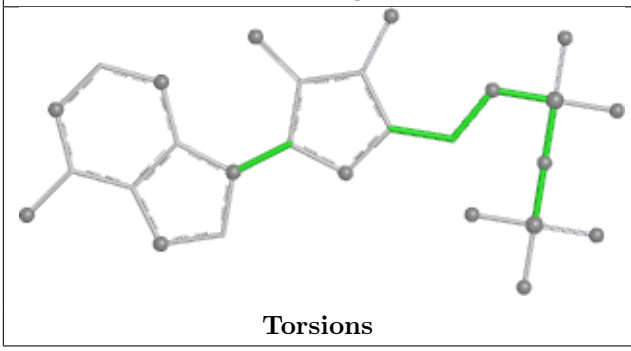
Ligand ADP A 4704



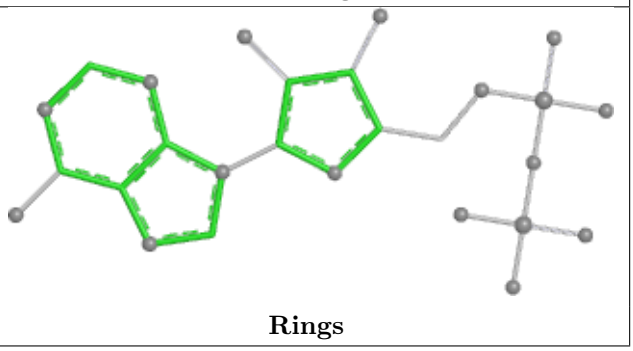
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

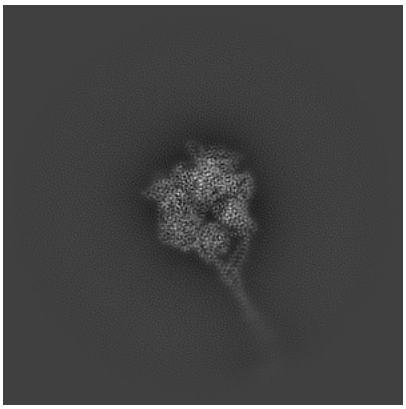
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44699. These allow visual inspection of the internal detail of the map and identification of artifacts.

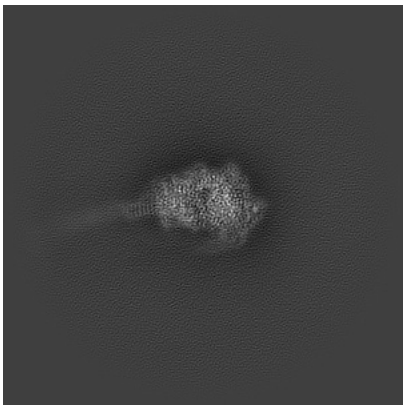
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

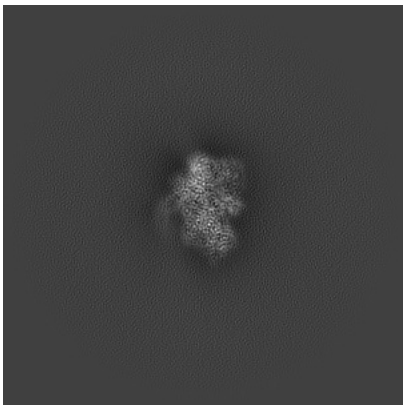
6.1.1 Primary map



X

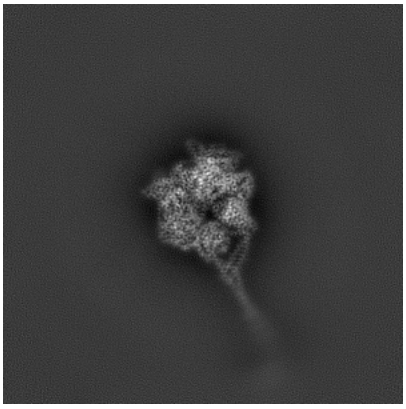


Y



Z

6.1.2 Raw map



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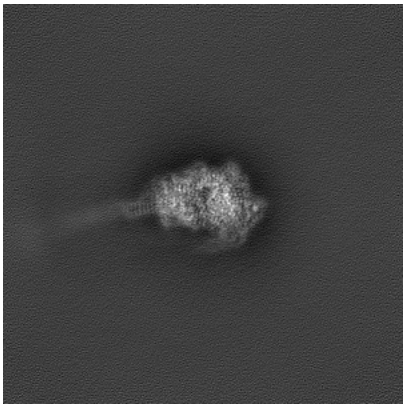
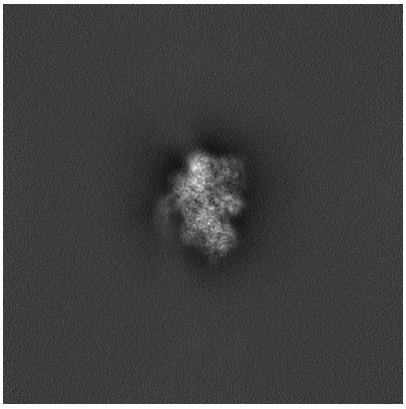


Y

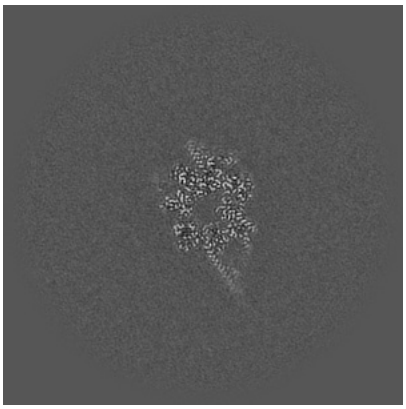


Z

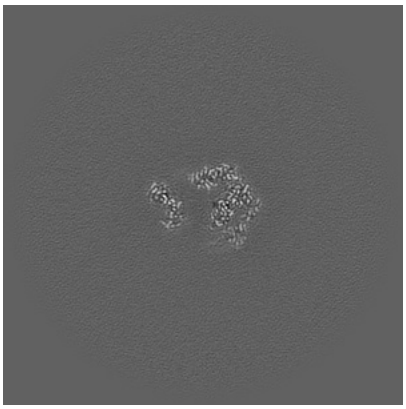
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

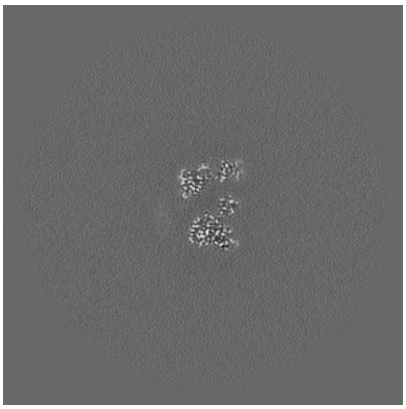
6.2.1 Primary map



X Index: 192

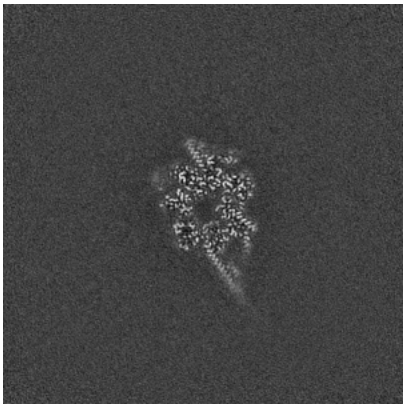


Y Index: 192

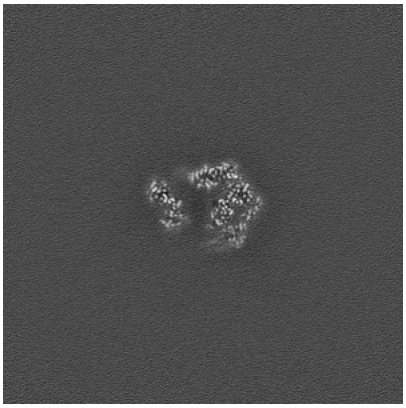


Z Index: 192

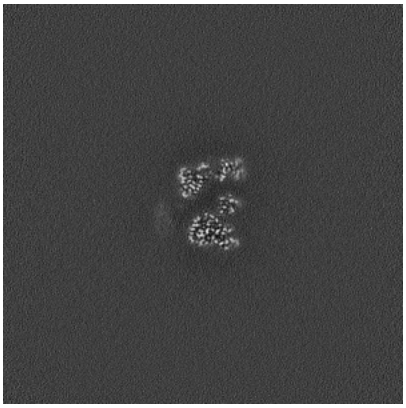
6.2.2 Raw map



X Index: 192



Y Index: 192

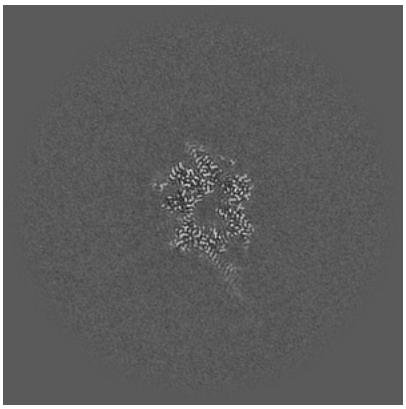


Z Index: 192

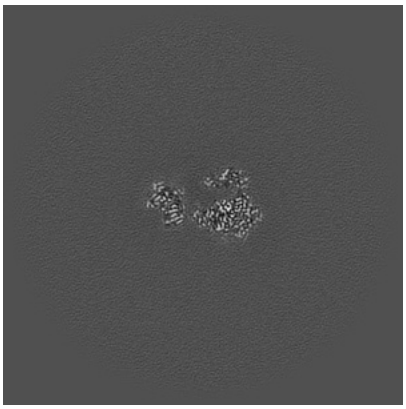
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

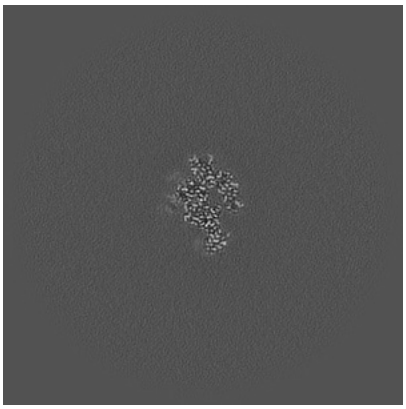
6.3.1 Primary map



X Index: 194

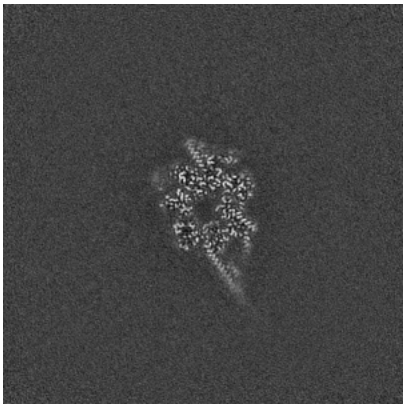


Y Index: 201

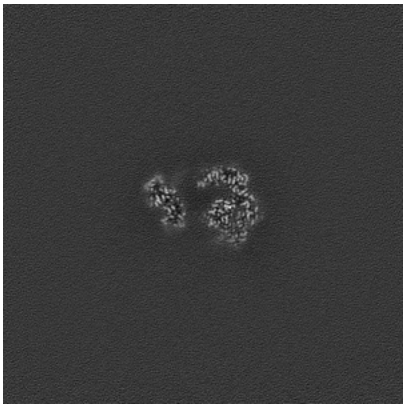


Z Index: 213

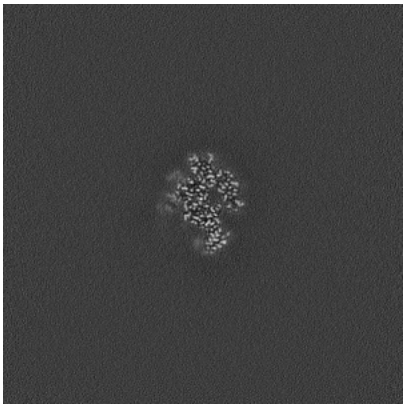
6.3.2 Raw map



X Index: 192



Y Index: 197

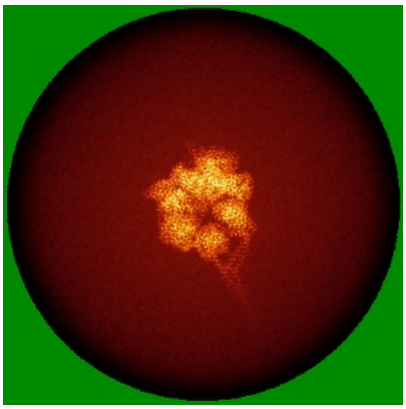


Z Index: 213

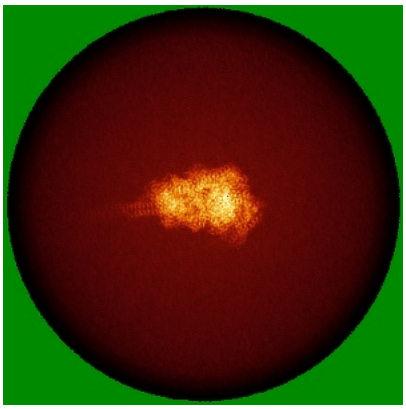
The images above show the largest variance slices of the map in three orthogonal directions.

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

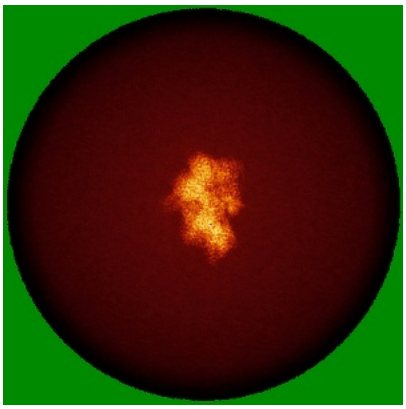
6.4.1 Primary map



X

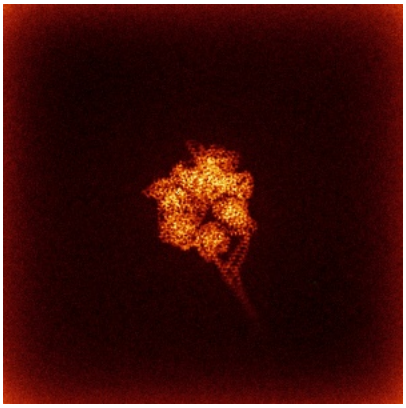


Y

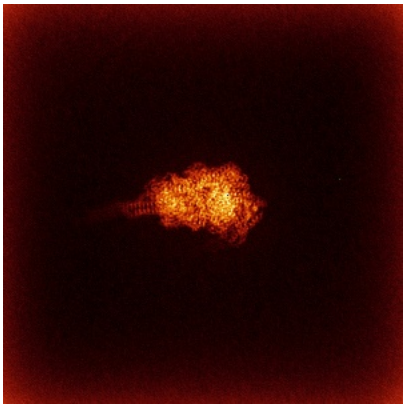


Z

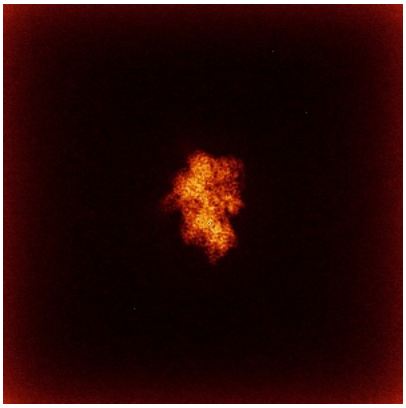
6.4.2 Raw map



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 0.3. 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.

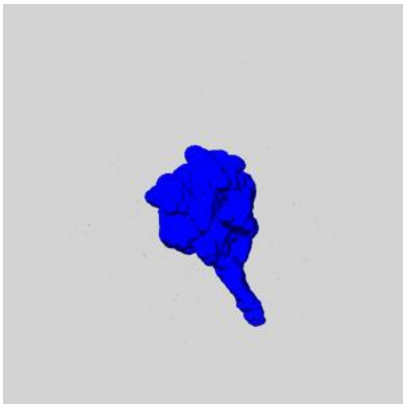
6.6 Mask visualisation

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

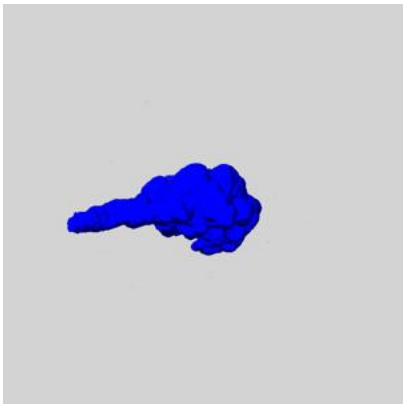
A mask typically either:

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

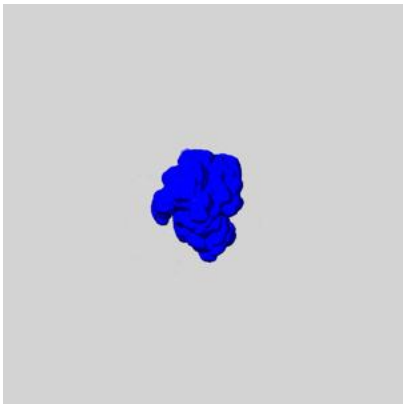
6.6.1 emd_44699_msk_1.map



X



Y

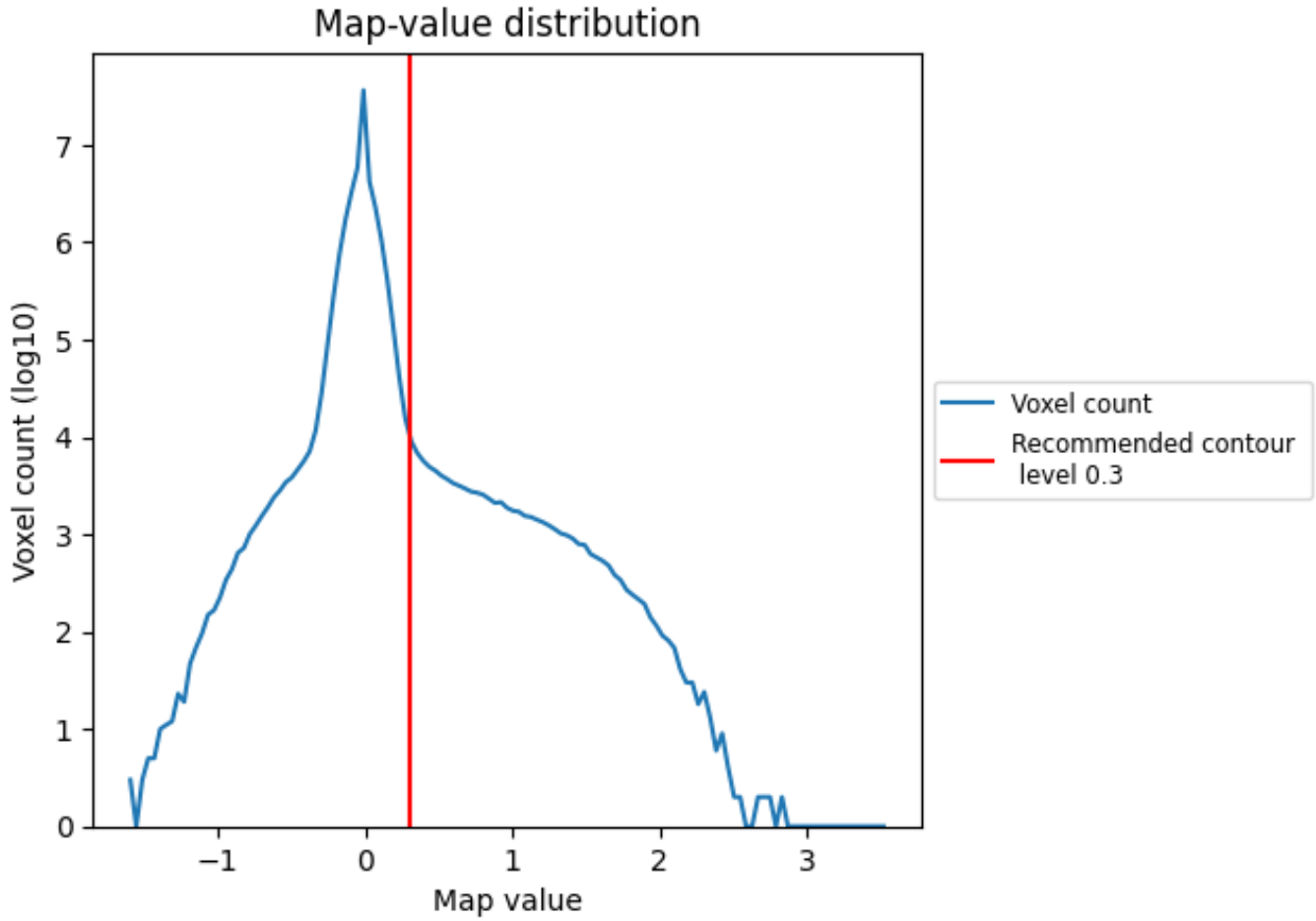


Z

7 Map analysis

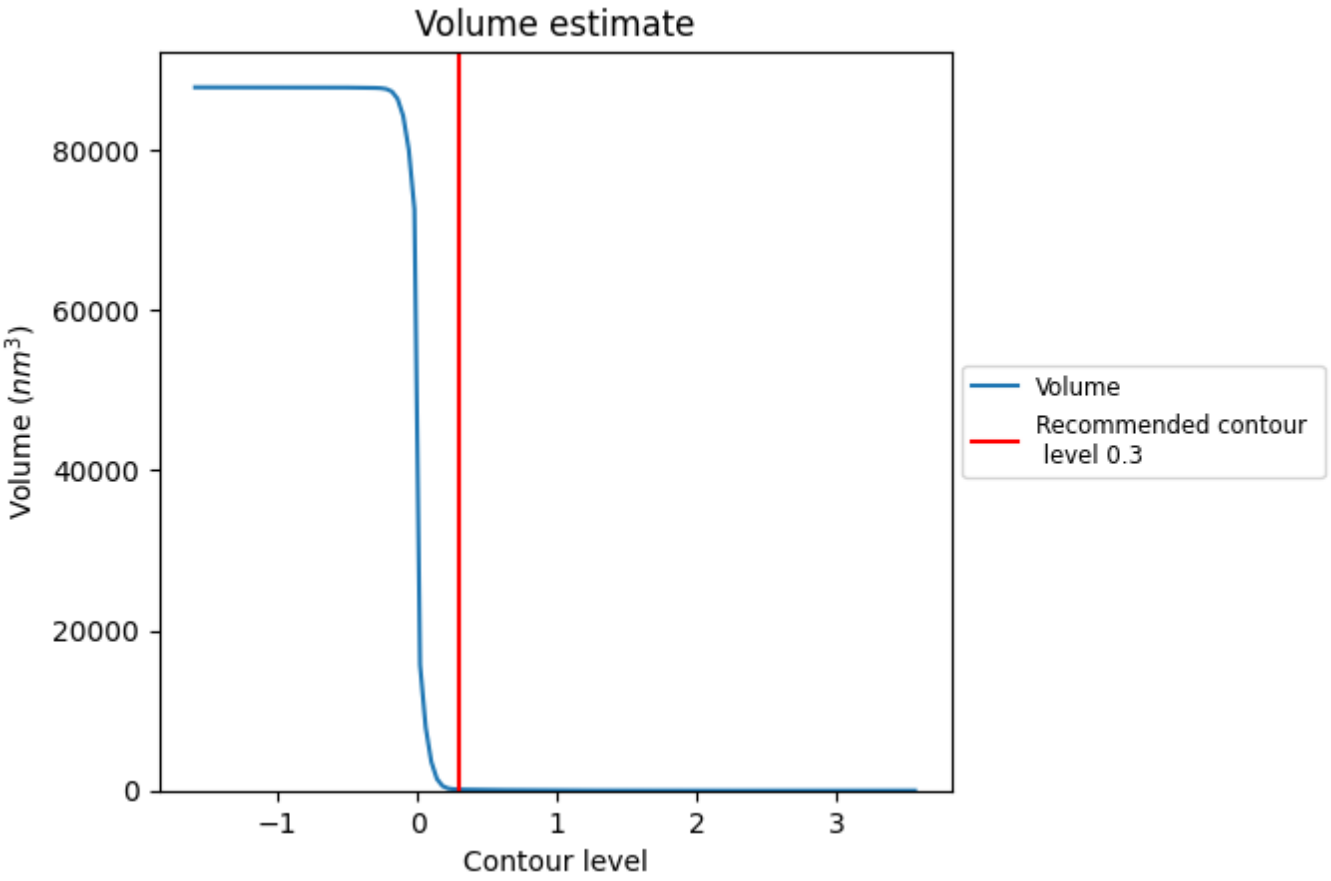
This section contains the results of statistical analysis of the map.

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.

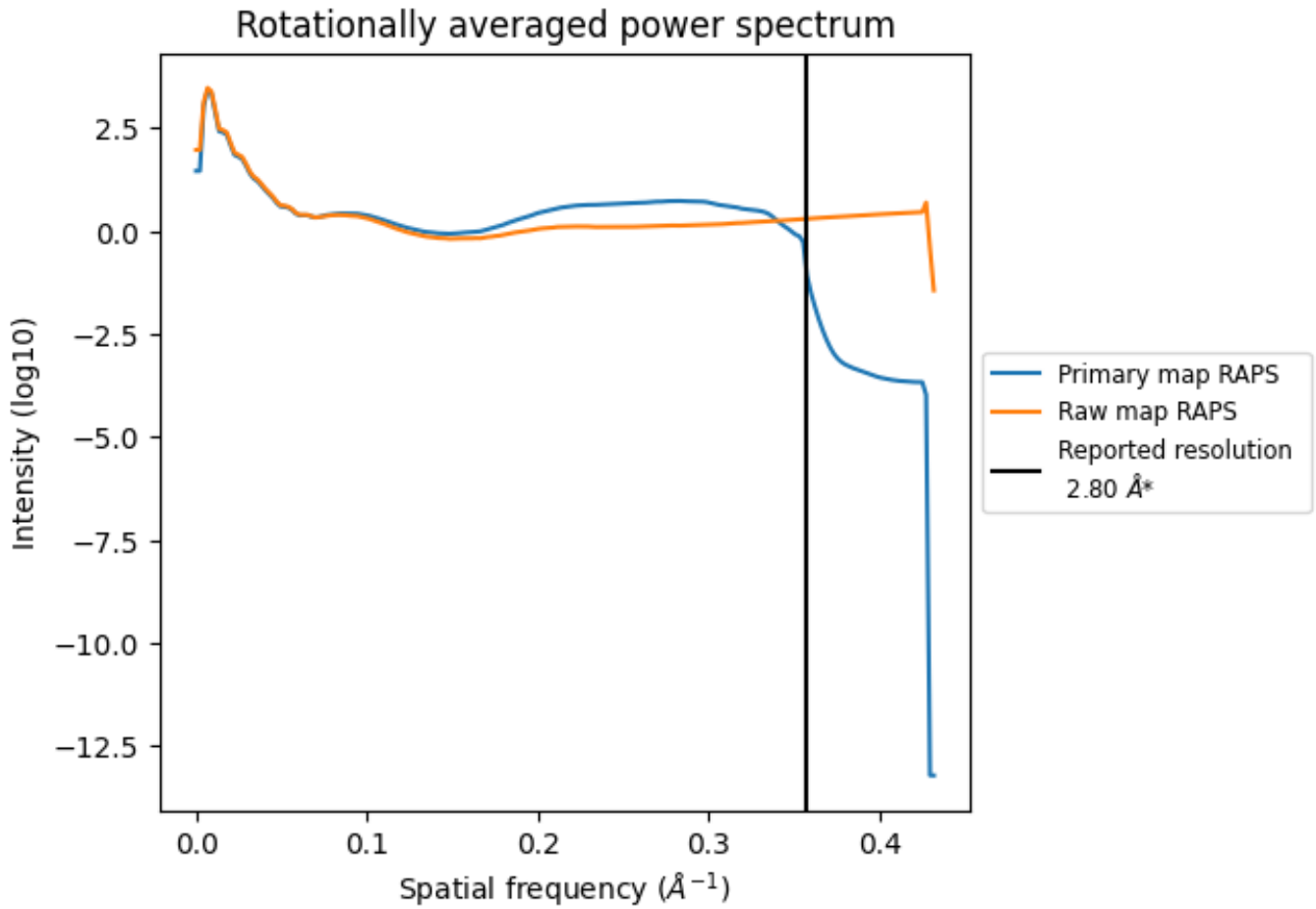
7.2 Volume estimate



The volume at the recommended contour level is 138 nm^3; this corresponds to an approximate mass of 125 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)

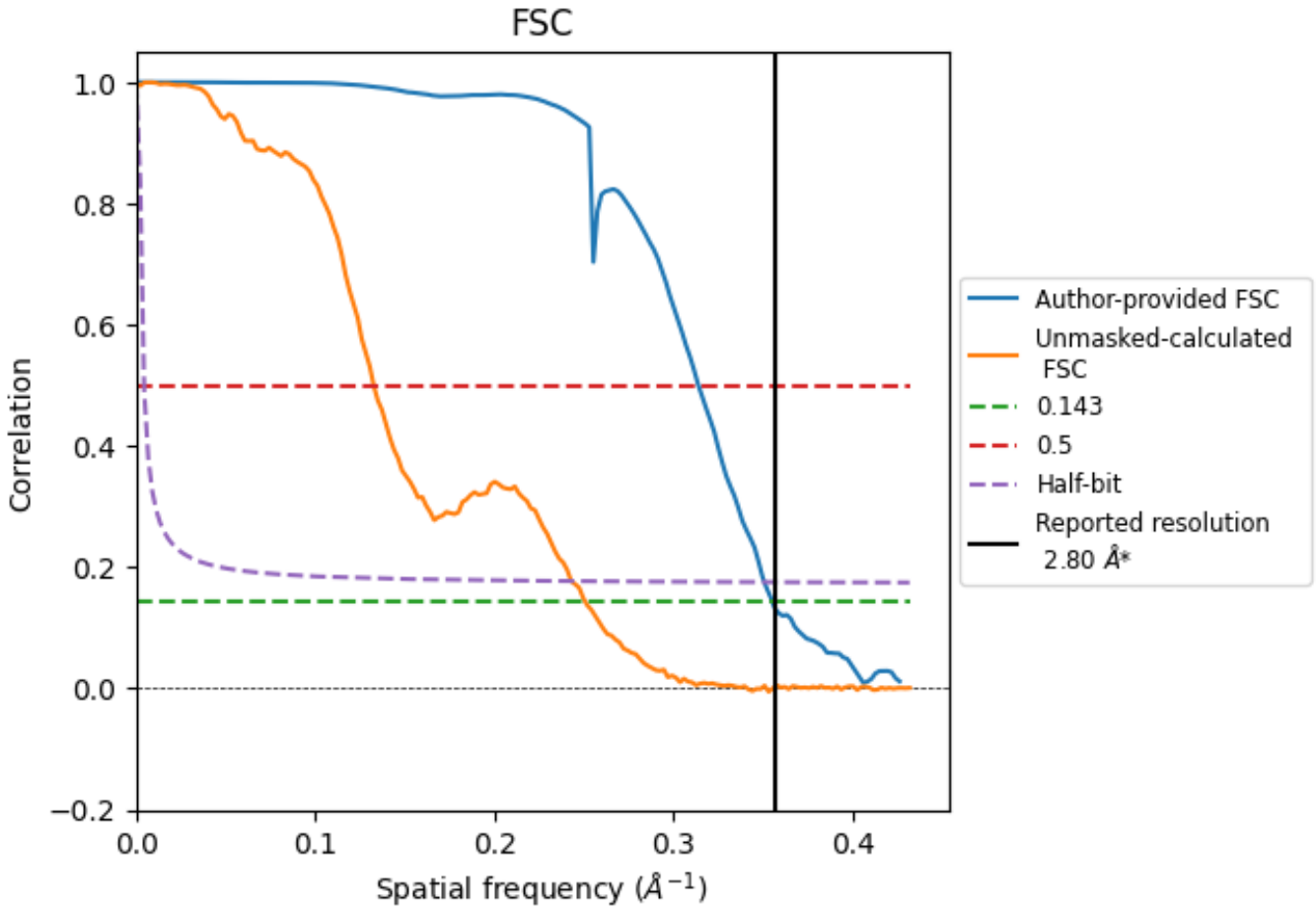


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

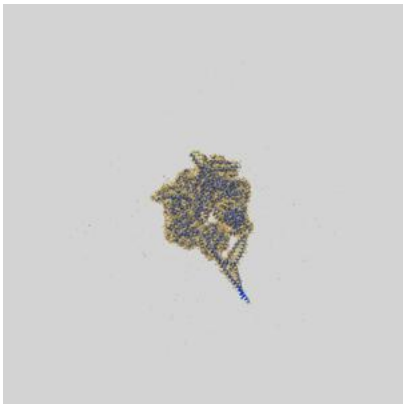
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.81	3.18	2.85
Unmasked-calculated*	3.99	7.54	4.12

*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 3.99 differs from the reported value 2.8 by more than 10 %

9 Map-model fit

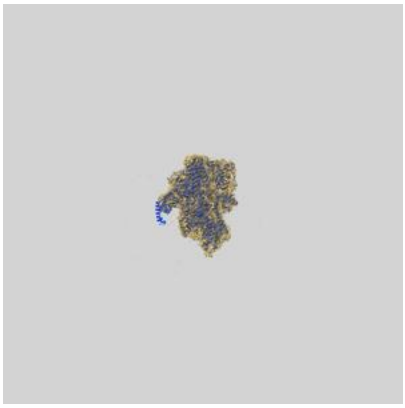
This section contains information regarding the fit between EMDB map EMD-44699 and PDB model 9BMH. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay



X

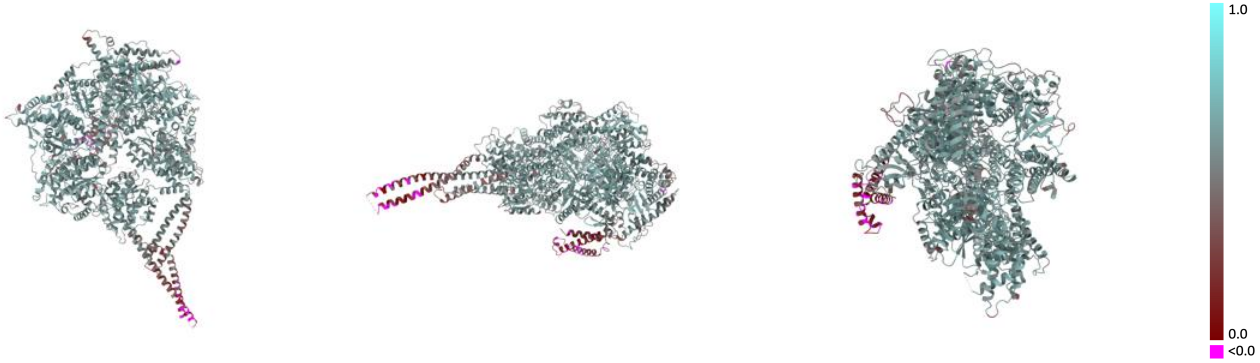
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

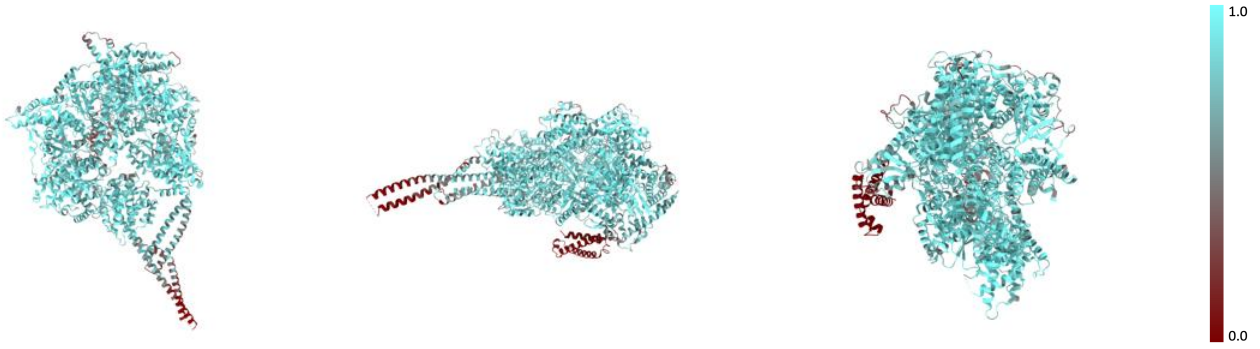
9.2 Q-score mapped to coordinate model (i)



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.

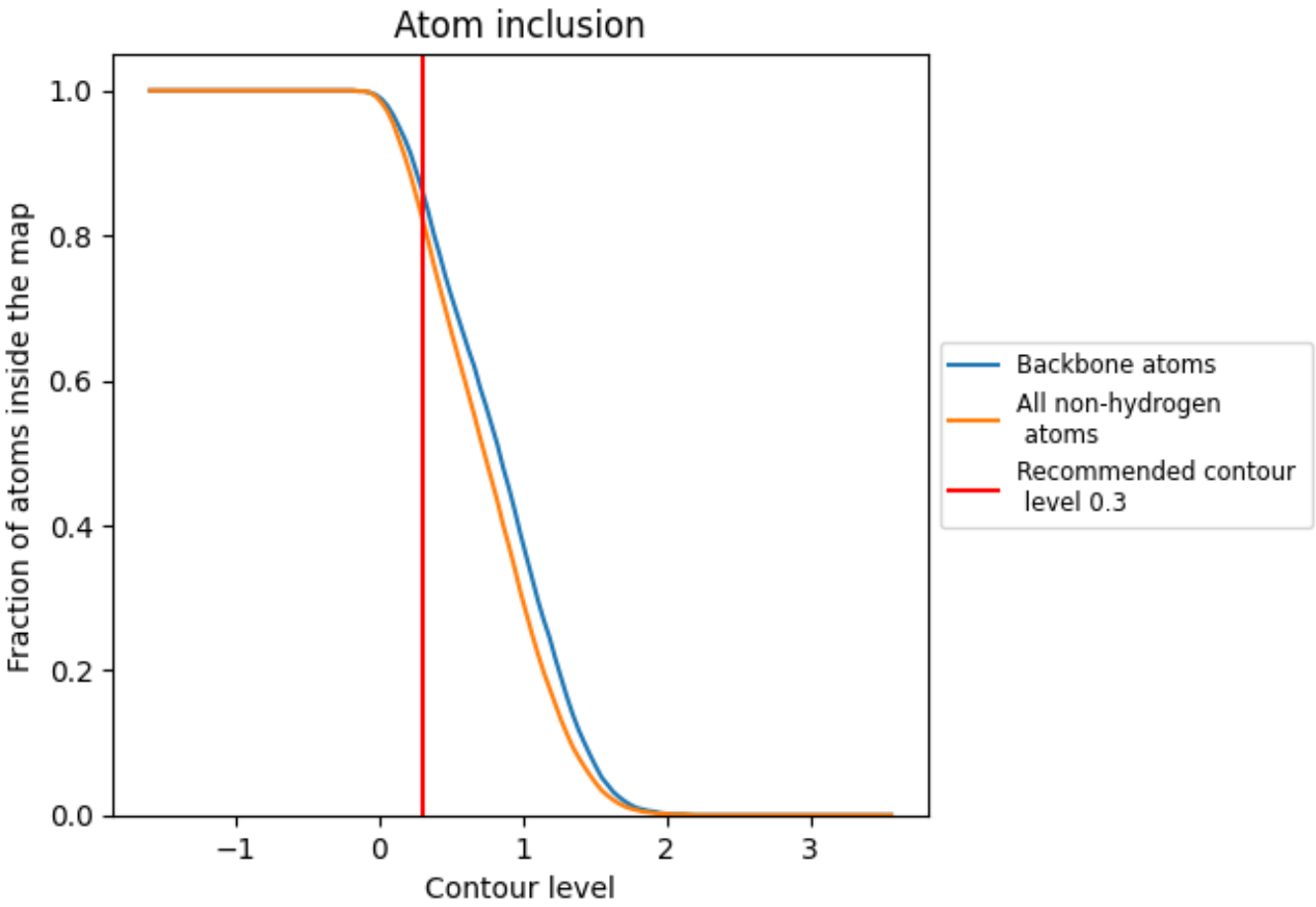
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.5530
A	0.8240	0.5530