



## Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 07:42 PM EST

PDB ID : 3JBZ  
EMDB ID : EMD-6501  
Title : Crystal structure of mTOR docked into EM map of dimeric ATM kinase  
Authors : Lau, W.C.Y.  
Deposited on : 2015-11-03  
Resolution : 28.00 Å(reported)  
Based on initial model : 4JSV

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

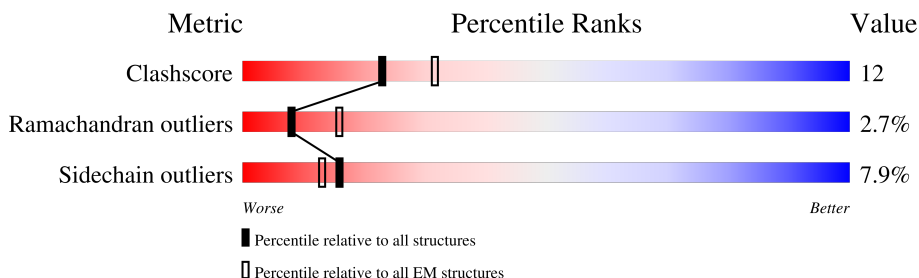
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 28.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1165	<div> <div>5%</div> <div>57%</div> <div>22%</div> <div>•</div> <div>18%</div> </div>

## 2 Entry composition [i](#)

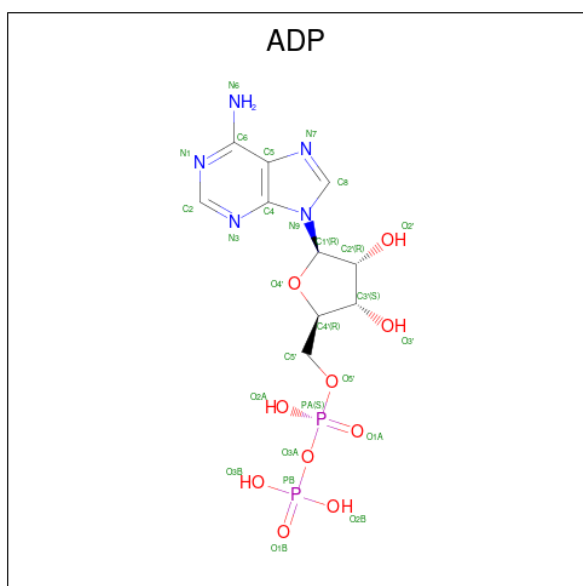
There are 4 unique types of molecules in this entry. The entry contains 7808 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	960	Total	C	N	O	S	0	0
			7775	4939	1375	1405	56		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

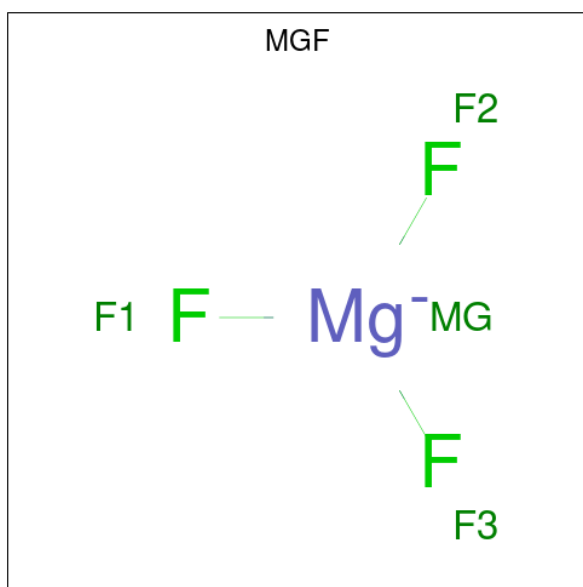


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

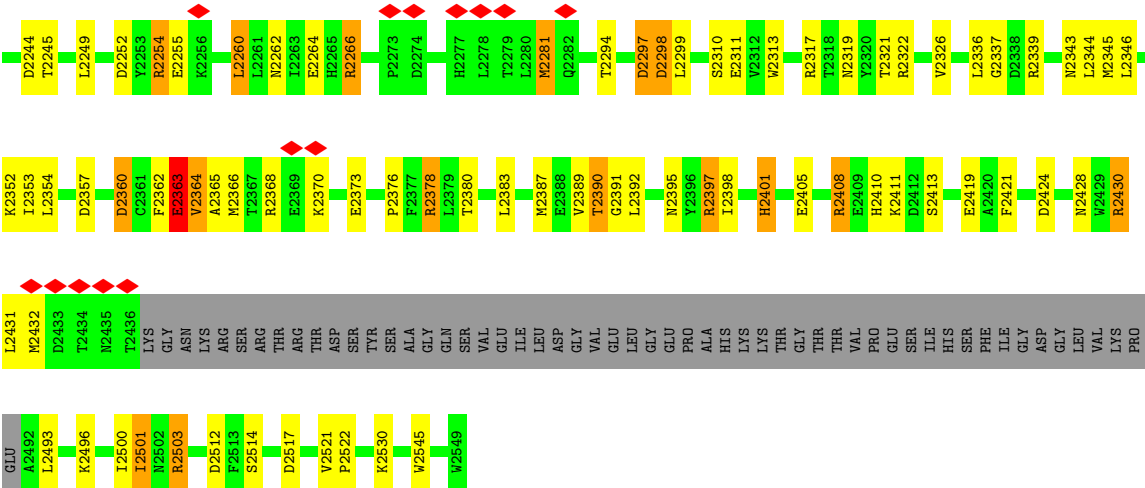
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Mg	0
			2	2	

- Molecule 4 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula:  $F_3Mg$ ).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	F	Mg	0
			4	3	1	





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL 2010	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	50000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	1.953	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.143	Depositor
Recommended contour level	0.9	Depositor
Map size ( $\text{\AA}$ )	461.0, 461.0, 461.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	4.61, 4.61, 4.61	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MGF, 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	0.33	0/7947	0.57	0/10763

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1914	GLY	Peptide

### 5.2 Too-close contacts [i](#)

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	7775	0	7787	193	0
2	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
4	A	4	0	0	0	0
All	All	7808	0	7799	193	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 12.

All (193) 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:1969:PRO:O	1:A:1970:GLN:HB2	1.69	0.92
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.50	0.91
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.56	0.86
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.79	0.81
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.59	0.81
1:A:2392:LEU:O	1:A:2397:ARG:HB2	1.84	0.78
1:A:2357:ASP:OD2	2:A:2601:ADP:O3B	2.04	0.76
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.51	0.75
1:A:2401:HIS:O	1:A:2405:GLU:HB2	1.86	0.74
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	1.86	0.74
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.70	0.74
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.71	0.73
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.70	0.72
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.72	0.72
1:A:2266:ARG:HH11	1:A:2266:ARG:HB2	1.54	0.71
1:A:2223:GLN:HE22	1:A:2352:LYS:HB2	1.57	0.69
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.24	0.69
1:A:1990:ALA:HA	1:A:1993:LYS:HD2	1.74	0.69
1:A:2178:ASN:HD22	1:A:2179:GLY:N	1.91	0.69
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.58	0.68
1:A:1916:TRP:H	1:A:1916:TRP:HD1	1.38	0.68
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.59	0.68
1:A:1680:ASP:C	1:A:1682:SER:H	1.97	0.68
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.77	0.67
1:A:1732:ILE:HD13	1:A:1740:LYS:HD2	1.77	0.66
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.78	0.66
1:A:1915:HIS:CD2	1:A:1953:VAL:HG22	2.30	0.65
1:A:1980:SER:O	1:A:1988:HIS:HB2	1.96	0.65
1:A:1583:TYR:C	1:A:1585:ARG:H	1.98	0.65
1:A:1417:ILE:HG23	1:A:1432:VAL:HB	1.79	0.65
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2281:MET:HE3	1:A:2281:MET:HA	1.81	0.63
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.31	0.63
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.81	0.62
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.81	0.61
1:A:1701:MET:HE1	1:A:1717:MET:N	2.15	0.61
1:A:1977:THR:HG21	1:A:2013:SER:OG	2.00	0.61
1:A:1771:LYS:O	1:A:1774:GLN:HB3	2.01	0.60
1:A:2419:GLU:HA	1:A:2501:ILE:HD11	1.83	0.60
1:A:1733:ALA:O	1:A:1735:GLU:N	2.36	0.59
1:A:1680:ASP:C	1:A:1682:SER:N	2.55	0.59
1:A:2281:MET:HA	1:A:2281:MET:CE	2.32	0.59
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.15	0.59
1:A:2178:ASN:HD22	1:A:2179:GLY:H	1.50	0.59
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.03	0.58
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.38	0.57
1:A:1783:ASP:O	1:A:1785:SER:N	2.37	0.57
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.87	0.57
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.87	0.56
1:A:2163:ILE:HB	1:A:2169:PRO:HG2	1.87	0.56
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.87	0.56
1:A:1505:ASN:HB2	1:A:1508:THR:HB	1.87	0.56
1:A:2390:THR:HG23	1:A:2390:THR:O	2.06	0.56
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.06	0.55
1:A:1466:LYS:O	1:A:1470:ASN:HB2	2.06	0.55
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.04	0.55
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.71	0.55
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.71	0.55
1:A:1784:ARG:O	1:A:1790:TRP:NE1	2.38	0.55
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.05	0.55
1:A:1680:ASP:OD2	1:A:1683:ARG:HB2	2.07	0.54
1:A:1401:GLU:OE1	1:A:2317:ARG:NH1	2.40	0.54
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.28	0.54
1:A:1913:TYR:O	1:A:1915:HIS:ND1	2.41	0.53
1:A:1916:TRP:CD1	1:A:1916:TRP:N	2.64	0.53
1:A:2336:LEU:HG	1:A:2339:ARG:HH11	1.72	0.53
1:A:1557:PHE:CE2	1:A:1606:LYS:HB3	2.44	0.52
1:A:1701:MET:HE1	1:A:1717:MET:CA	2.38	0.52
1:A:2368:ARG:HD2	1:A:2370:LYS:O	2.10	0.52
1:A:1457:GLU:HG2	1:A:1487:LEU:HD21	1.92	0.52
1:A:1999:CYS:HA	1:A:2003:ASN:HA	1.92	0.51
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.45	0.51
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.91	0.51
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.92	0.51
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.93	0.50
1:A:1943:ILE:CD1	1:A:1975:PRO:HB2	2.41	0.50
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	1.94	0.50
1:A:1717:MET:HG3	1:A:1754:LEU:HG	1.94	0.50
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.94	0.50
1:A:1437:MET:SD	1:A:1453:LEU:HD11	2.52	0.49
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.12	0.49
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.93	0.49
1:A:1933:ASP:O	1:A:1934:THR:C	2.50	0.49
1:A:1943:ILE:O	1:A:1946:ILE:HG13	2.12	0.49
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.94	0.49
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.94	0.49
1:A:1892:ILE:CG2	1:A:1930:ILE:HD11	2.39	0.49
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.13	0.49
1:A:1895:SER:CB	1:A:1899:ASN:HB3	2.41	0.49
1:A:1497:CYS:SG	1:A:1516:ALA:HB2	2.52	0.48
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.47	0.48
1:A:1807:GLN:O	1:A:1811:ARG:HG2	2.13	0.48
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.46	0.48
1:A:2345:MET:HG3	1:A:2354:LEU:HD23	1.93	0.48
1:A:1752:LEU:O	1:A:1756:GLU:HB2	2.14	0.48
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.50	0.48
1:A:2321:THR:HG23	1:A:2387:MET:HG2	1.94	0.48
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.78	0.48
1:A:1747:MET:O	1:A:1750:CYS:HB2	2.14	0.48
1:A:2366:MET:HG2	1:A:2373:GLU:O	2.13	0.48
1:A:1583:TYR:C	1:A:1585:ARG:N	2.67	0.48
1:A:1496:GLN:NE2	1:A:1500:LYS:HG3	2.29	0.47
1:A:1734:THR:O	1:A:1736:ASP:N	2.47	0.47
1:A:1876:THR:O	1:A:1879:MET:HB3	2.14	0.47
1:A:1508:THR:O	1:A:1512:MET:HB2	2.14	0.47
1:A:1982:SER:OG	1:A:1984:THR:HG23	2.14	0.47
1:A:1797:ASN:HB3	1:A:1884:ALA:HB2	1.97	0.47
1:A:2154:GLN:NE2	1:A:2155:SER:HB2	2.30	0.47
1:A:2336:LEU:HG	1:A:2339:ARG:NH1	2.30	0.47
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.96	0.47
1:A:2310:SER:HA	1:A:2313:TRP:HB3	1.95	0.47
1:A:2363:GLU:O	1:A:2366:MET:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1433:LEU:HD21	1:A:1452:LYS:HB3	1.98	0.46
1:A:2156:ILE:HG12	1:A:2174:LEU:HD22	1.97	0.46
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.32	0.46
1:A:1936:LEU:HD23	1:A:1939:ILE:HD11	1.98	0.46
1:A:1415:SER:O	1:A:1419:ILE:HG22	2.16	0.46
1:A:1734:THR:C	1:A:1736:ASP:H	2.18	0.46
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.81	0.46
1:A:2208:LEU:HD22	1:A:2410:HIS:CD2	2.51	0.46
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.97	0.45
1:A:1433:LEU:HD23	1:A:1453:LEU:HD23	1.98	0.45
1:A:2123:LEU:HB2	1:A:2158:PRO:O	2.17	0.45
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.49	0.45
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.17	0.45
1:A:1574:GLU:HG2	1:A:1585:ARG:NH2	2.32	0.45
1:A:2363:GLU:OE2	1:A:2503:ARG:NH1	2.49	0.45
1:A:2421:PHE:CD1	1:A:2430:ARG:NH2	2.85	0.45
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.32	0.45
1:A:2004:THR:HA	1:A:2007:GLN:HB2	1.99	0.45
1:A:1608:VAL:O	1:A:1608:VAL:HG23	2.15	0.45
1:A:1973:ILE:HD13	1:A:2005:LEU:HD22	1.99	0.45
1:A:2322:ARG:O	1:A:2326:VAL:HG23	2.17	0.45
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.17	0.44
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.44
1:A:1427:GLU:HB2	1:A:2398:ILE:CD1	2.48	0.44
1:A:1785:SER:O	1:A:1786:TRP:CB	2.65	0.44
1:A:2167:GLN:CG	1:A:2189:HIS:CD2	3.00	0.44
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	1.98	0.44
1:A:1744:HIS:O	1:A:1782:HIS:HB3	2.17	0.44
1:A:1649:ASP:HB3	1:A:1653:TRP:HD1	1.81	0.44
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.53	0.44
1:A:1631:GLU:H	1:A:1631:GLU:CD	2.20	0.44
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.18	0.44
1:A:2297:ASP:O	1:A:2299:LEU:N	2.51	0.44
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.18	0.44
1:A:2319:ASN:HD22	1:A:2352:LYS:HG3	1.82	0.43
1:A:1796:MET:HA	1:A:1796:MET:CE	2.48	0.43
1:A:1992:ASN:HA	1:A:1995:LEU:HD12	2.00	0.43
1:A:2339:ARG:HH21	1:A:2343:ASN:HB3	1.83	0.43
1:A:1896:ARG:NH2	1:A:1933:ASP:OD2	2.52	0.43
1:A:2430:ARG:H	1:A:2430:ARG:HG3	1.69	0.43
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2249:LEU:HD13	1:A:2346:LEU:HD12	2.00	0.43
1:A:1899:ASN:ND2	1:A:1937:GLN:HE22	2.17	0.43
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.72	0.43
1:A:1697:THR:O	1:A:1701:MET:HG3	2.18	0.43
1:A:1505:ASN:O	1:A:1509:GLN:HB2	2.19	0.42
1:A:2129:LYS:O	1:A:2132:MET:HB3	2.19	0.42
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.20	0.42
1:A:2223:GLN:HE22	1:A:2352:LYS:CB	2.30	0.42
1:A:1727:GLN:O	1:A:1731:ALA:HB3	2.19	0.42
1:A:1777:SER:O	1:A:1781:GLU:HG2	2.20	0.42
1:A:1532:TYR:O	1:A:1536:ILE:HG13	2.19	0.42
1:A:1759:LEU:HD21	1:A:1772:VAL:HG21	2.00	0.42
1:A:1418:SER:HB2	1:A:1581:GLU:CG	2.39	0.42
1:A:1717:MET:CG	1:A:1754:LEU:HG	2.49	0.42
1:A:2362:PHE:O	1:A:2364:VAL:N	2.52	0.42
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.55	0.42
1:A:1939:ILE:N	1:A:1940:PRO:HD2	2.35	0.42
1:A:2167:GLN:CG	1:A:2189:HIS:HD2	2.31	0.42
1:A:2363:GLU:O	1:A:2365:ALA:N	2.53	0.41
1:A:1734:THR:C	1:A:1736:ASP:N	2.73	0.41
1:A:2360:ASP:N	1:A:2360:ASP:OD1	2.54	0.41
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	2.01	0.41
1:A:2319:ASN:ND2	1:A:2352:LYS:HE3	2.35	0.41
1:A:1973:ILE:H	1:A:1973:ILE:HG13	1.54	0.41
1:A:1477:MET:HE2	1:A:1477:MET:HB3	1.79	0.41
1:A:1916:TRP:HA	1:A:1917:PRO:HD2	1.65	0.41
1:A:2408:ARG:O	1:A:2411:LYS:HG2	2.21	0.41
1:A:2252:ASP:O	1:A:2255:GLU:HG2	2.21	0.41
1:A:1410:PRO:HA	1:A:1413:LEU:HB2	2.02	0.41
1:A:2009:ALA:HA	1:A:2138:LEU:HD11	2.01	0.41
1:A:2152:ARG:HG2	1:A:2177:SER:HB3	2.03	0.41
1:A:2254:ARG:HH22	1:A:2264:GLU:CD	2.24	0.41
1:A:1631:GLU:HA	1:A:1634:GLN:HE21	1.86	0.41
1:A:2378:ARG:HE	1:A:2378:ARG:HB2	1.67	0.41
1:A:1608:VAL:HA	1:A:1609:PRO:HD3	1.95	0.40
1:A:1895:SER:O	1:A:1896:ARG:C	2.59	0.40
1:A:2405:GLU:OE2	1:A:2521:VAL:HG21	2.22	0.40
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.85	0.40
1:A:2260:LEU:HD21	1:A:2266:ARG:CZ	2.52	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	952/1165 (82%)	847 (89%)	79 (8%)	26 (3%)	5	31

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1525	GLN
1	A	1611	ARG
1	A	1630	VAL
1	A	1650	MET
1	A	1734	THR
1	A	1970	GLN
1	A	2298	ASP
1	A	2364	VAL
1	A	1445	ILE
1	A	1735	GLU
1	A	1896	ARG
1	A	1914	GLY
1	A	1444	GLU
1	A	1784	ARG
1	A	1917	PRO
1	A	2363	GLU
1	A	1583	TYR
1	A	1709	ARG
1	A	1786	TRP
1	A	1934	THR
1	A	1584	SER
1	A	1681	PRO
1	A	1473	ASP
1	A	1680	ASP
1	A	2391	GLY
1	A	2376	PRO

### 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	844/1017 (83%)	777 (92%)	67 (8%)	12	35

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1457	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS
1	A	1590	MET
1	A	1605	TYR
1	A	1611	ARG
1	A	1630	VAL
1	A	1685	LEU
1	A	1724	MET
1	A	1736	ASP
1	A	1746	LEU
1	A	1780	THR
1	A	1872	ASP
1	A	1896	ARG
1	A	1899	ASN
1	A	1912	ASP
1	A	1916	TRP
1	A	1932	ILE
1	A	1938	VAL
1	A	1956	LEU
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2005	LEU
1	A	2011	MET

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Mol	Chain	Res	Type
1	A	2124	GLN
1	A	2138	LEU
1	A	2152	ARG
1	A	2154	GLN
1	A	2164	THR
1	A	2167	GLN
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2181	GLU
1	A	2185	LEU
1	A	2189	HIS
1	A	2195	ASP
1	A	2214	THR
1	A	2224	ARG
1	A	2228	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2260	LEU
1	A	2262	ASN
1	A	2266	ARG
1	A	2281	MET
1	A	2297	ASP
1	A	2311	GLU
1	A	2360	ASP
1	A	2363	GLU
1	A	2378	ARG
1	A	2390	THR
1	A	2397	ARG
1	A	2401	HIS
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2432	MET
1	A	2501	ILE
1	A	2503	ARG
1	A	2530	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1496	GLN

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Mol	Chain	Res	Type
1	A	1594	HIS
1	A	1670	HIS
1	A	1687	HIS
1	A	1695	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1898	ASN
1	A	1899	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1970	GLN
1	A	2154	GLN
1	A	2178	ASN
1	A	2189	HIS
1	A	2211	ASN
1	A	2223	GLN
1	A	2319	ASN
1	A	2340	HIS
1	A	2385	ASN
1	A	2395	ASN
1	A	2410	HIS
1	A	2502	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	2601	3,4	24,29,29	1.16	3 (12%)	29,45,45	1.20	3 (10%)
4	MGF	A	2604	2	0,3,3	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	2601	3,4	-	8/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2601	ADP	C5-C4	2.80	1.48	1.40
2	A	2601	ADP	O4'-C1'	2.76	1.44	1.41
2	A	2601	ADP	C2-N3	2.36	1.35	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2601	ADP	N3-C2-N1	-3.65	122.97	128.68
2	A	2601	ADP	C4-C5-N7	-2.20	107.10	109.40
2	A	2601	ADP	O3B-PB-O2B	2.07	115.54	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	ADP	C5'-O5'-PA-O1A
2	A	2601	ADP	O4'-C4'-C5'-O5'
2	A	2601	ADP	C4'-C5'-O5'-PA
2	A	2601	ADP	C3'-C4'-C5'-O5'
2	A	2601	ADP	C5'-O5'-PA-O3A
2	A	2601	ADP	PB-O3A-PA-O1A

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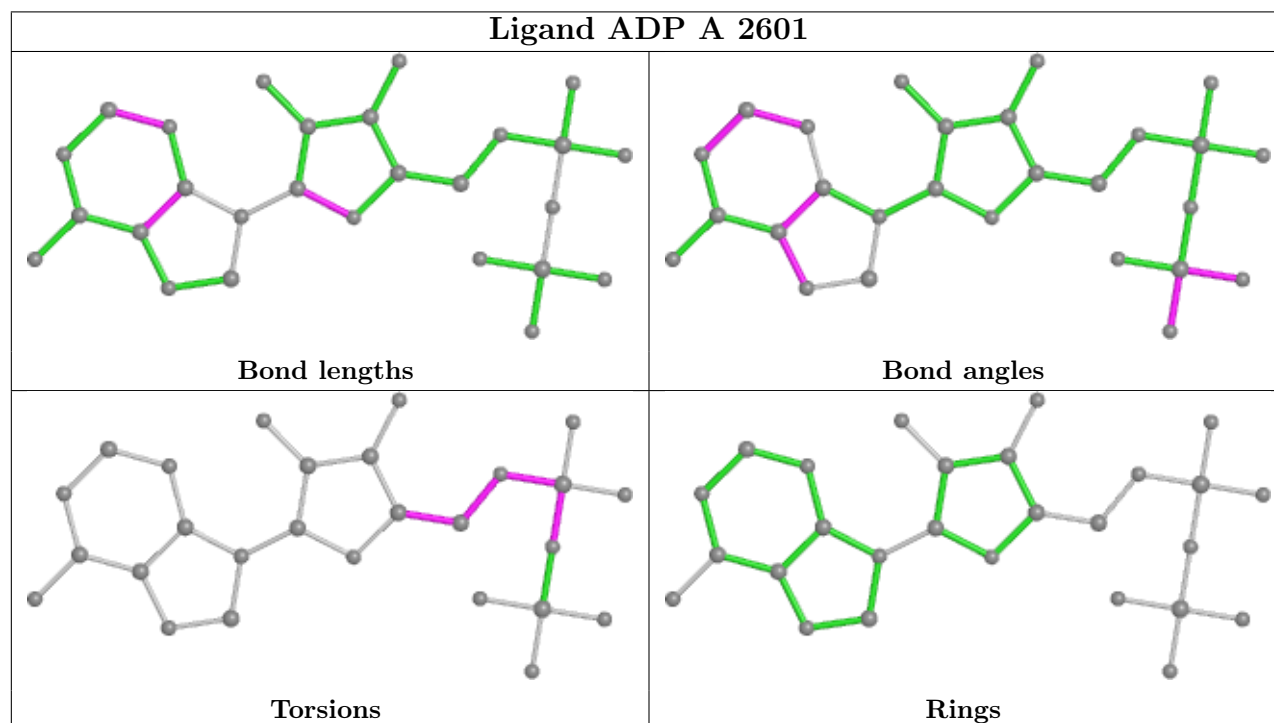
Mol	Chain	Res	Type	Atoms
2	A	2601	ADP	C5'-O5'-PA-O2A
2	A	2601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	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 than 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.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

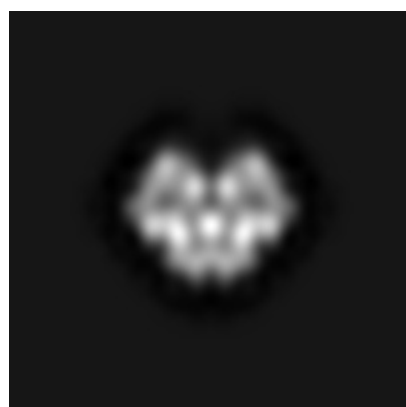
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6501. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

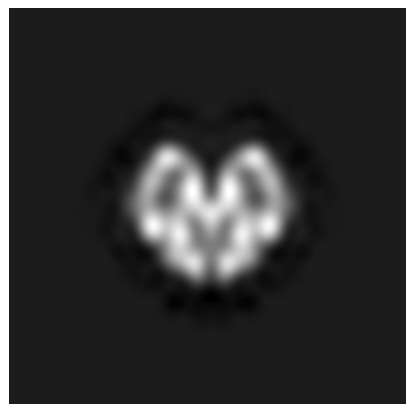


Z

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

### 6.2 Central slices [i](#)

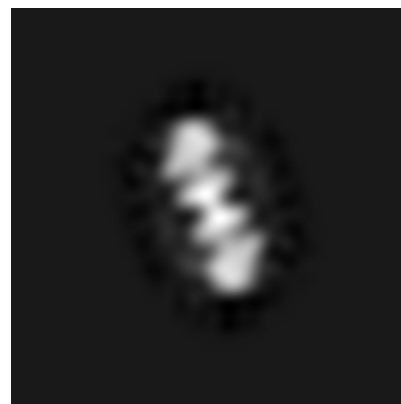
#### 6.2.1 Primary map



X Index: 50



Y Index: 50

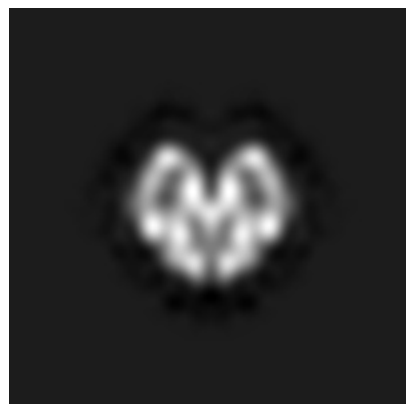


Z Index: 50

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: 50



Y Index: 42

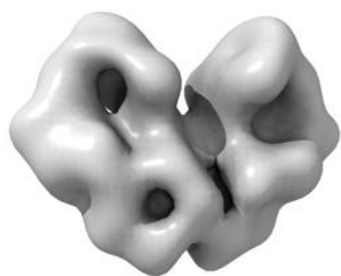


Z Index: 46

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

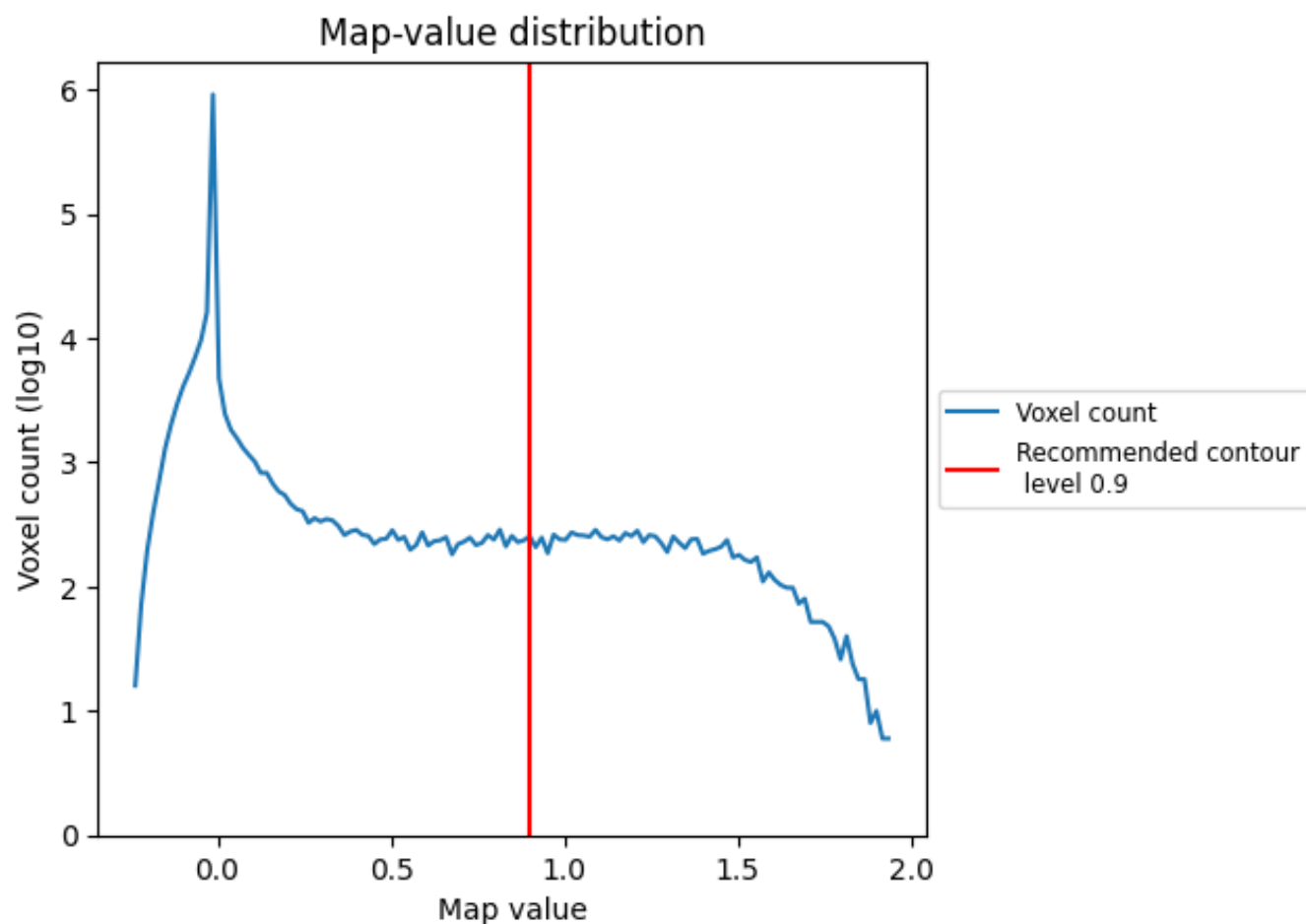
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

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

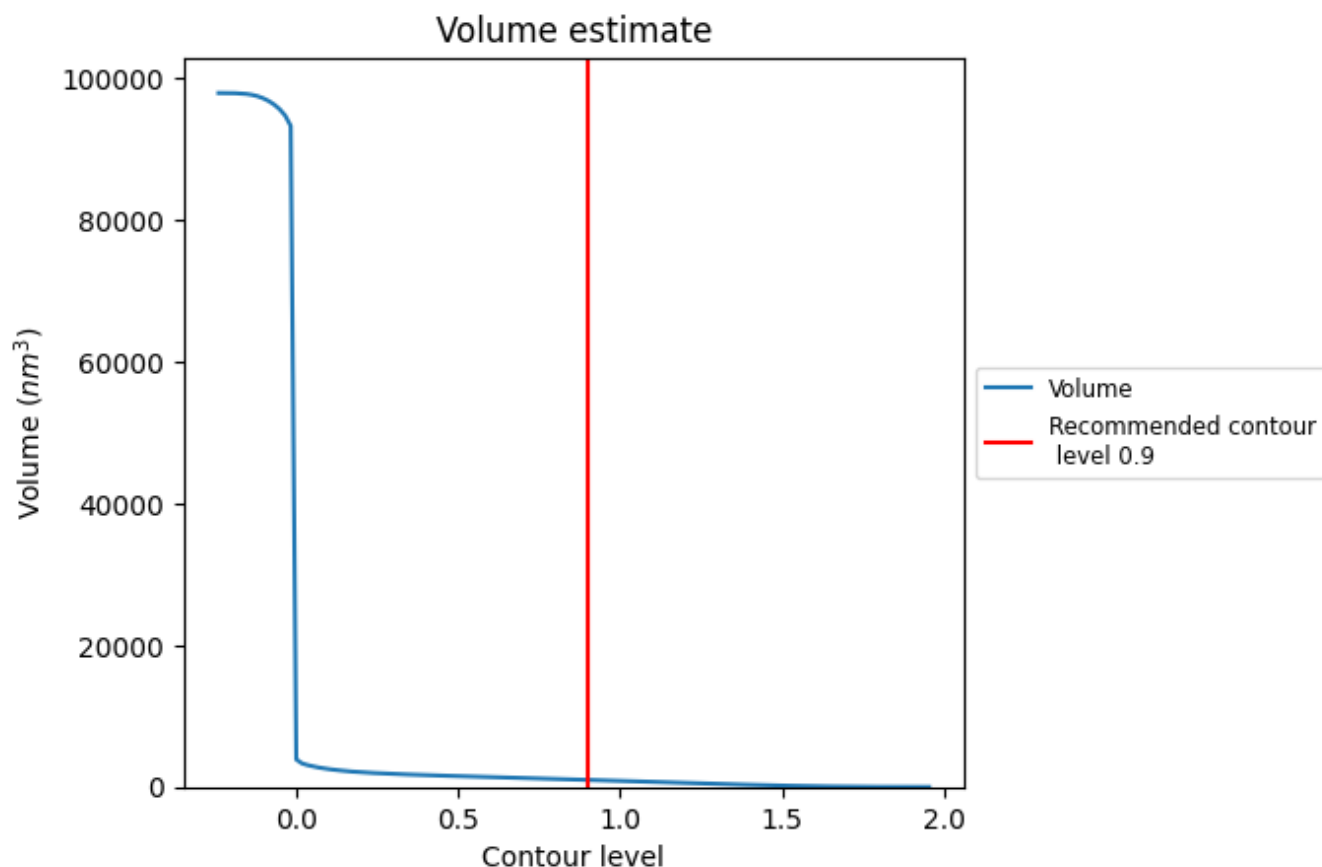
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



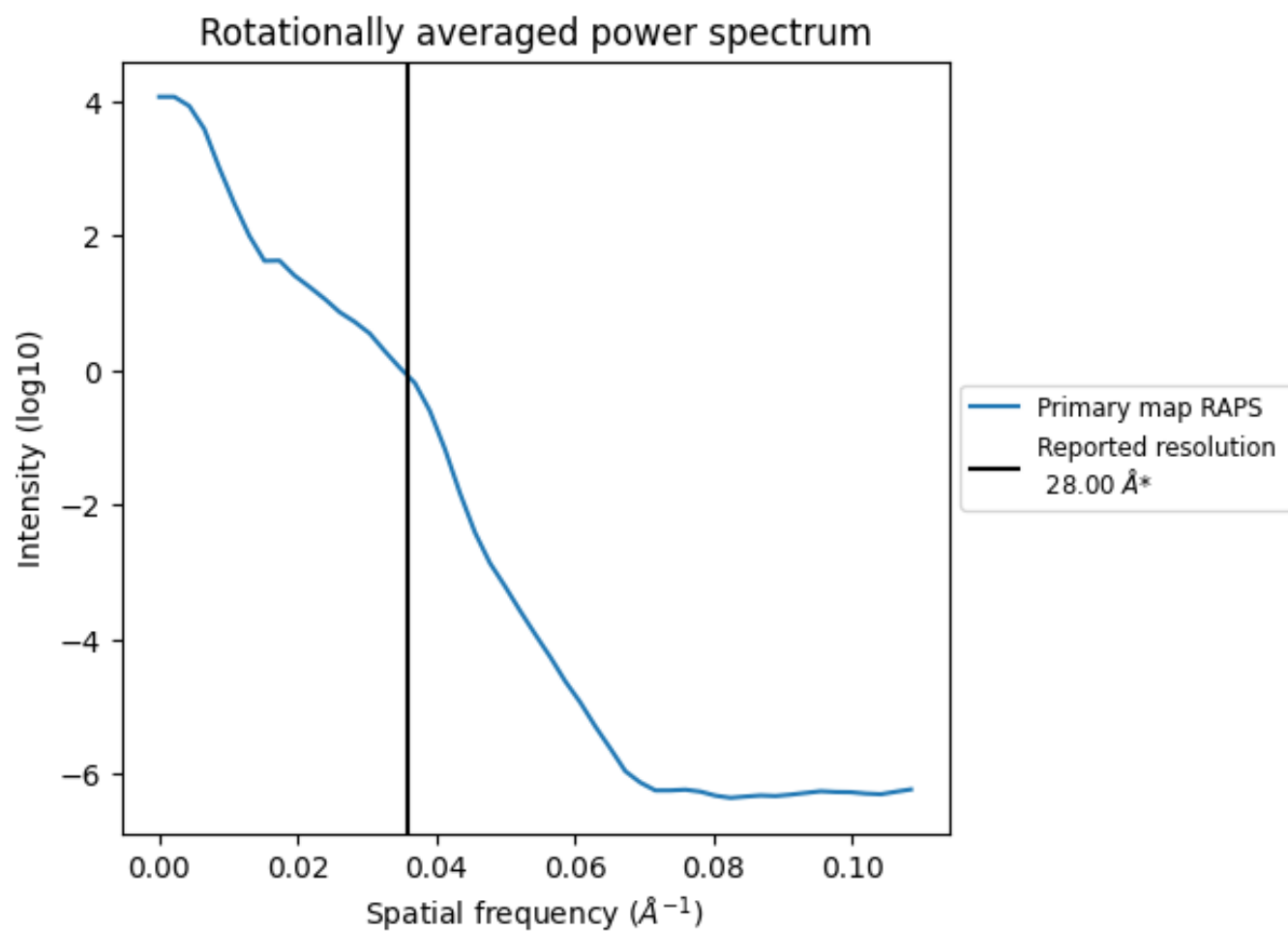
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 995  $\text{nm}^3$ ; this corresponds to an approximate mass of 899 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.036 Å<sup>-1</sup>

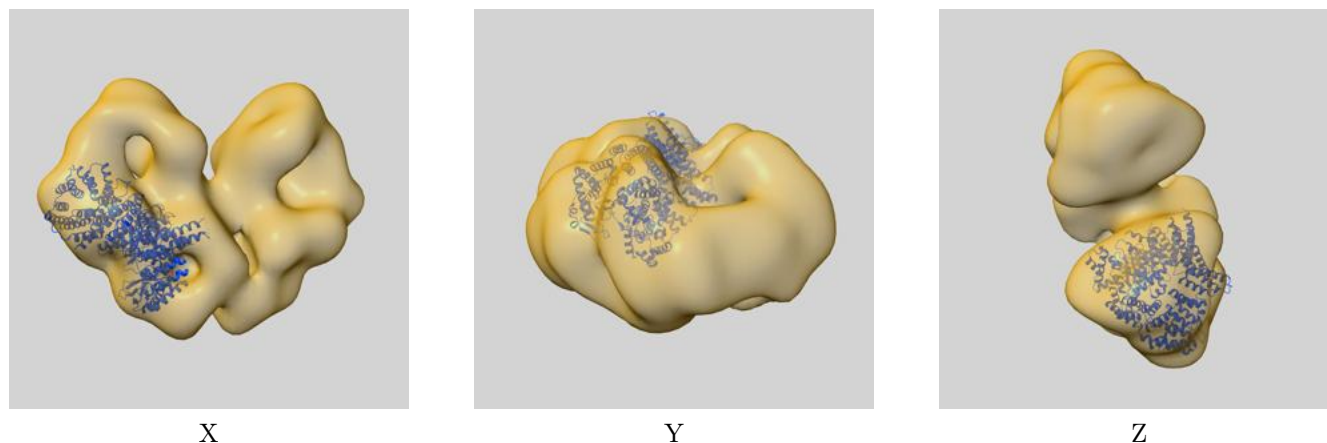
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

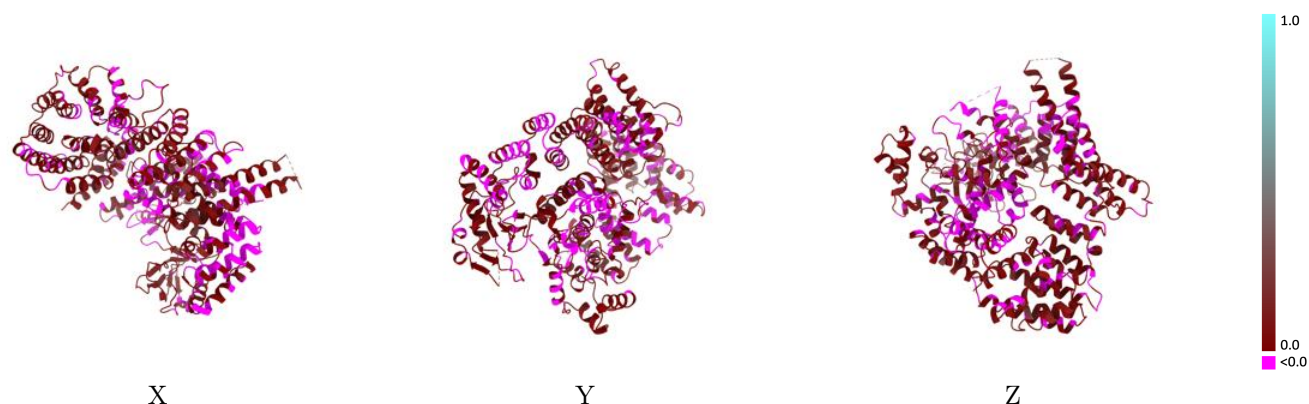
This section contains information regarding the fit between EMDB map EMD-6501 and PDB model 3JBZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



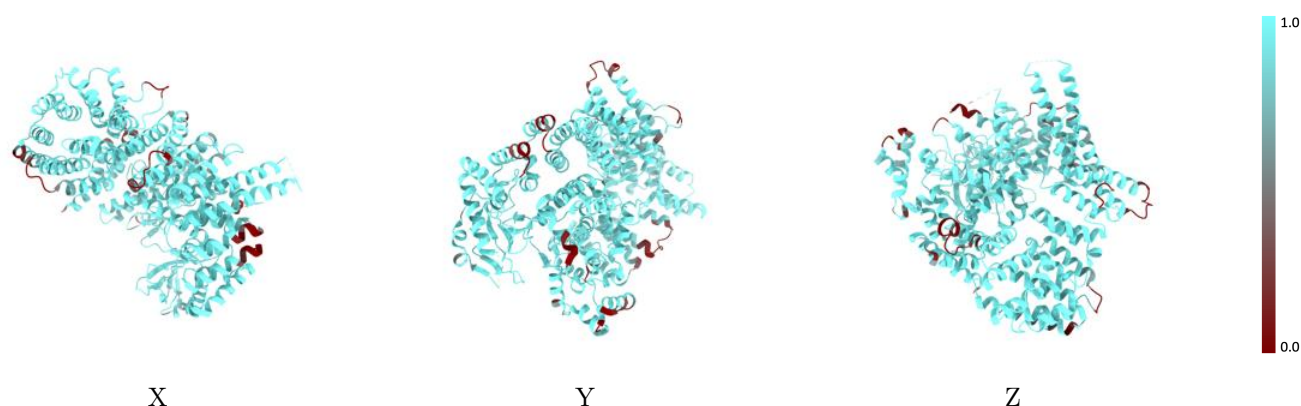
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



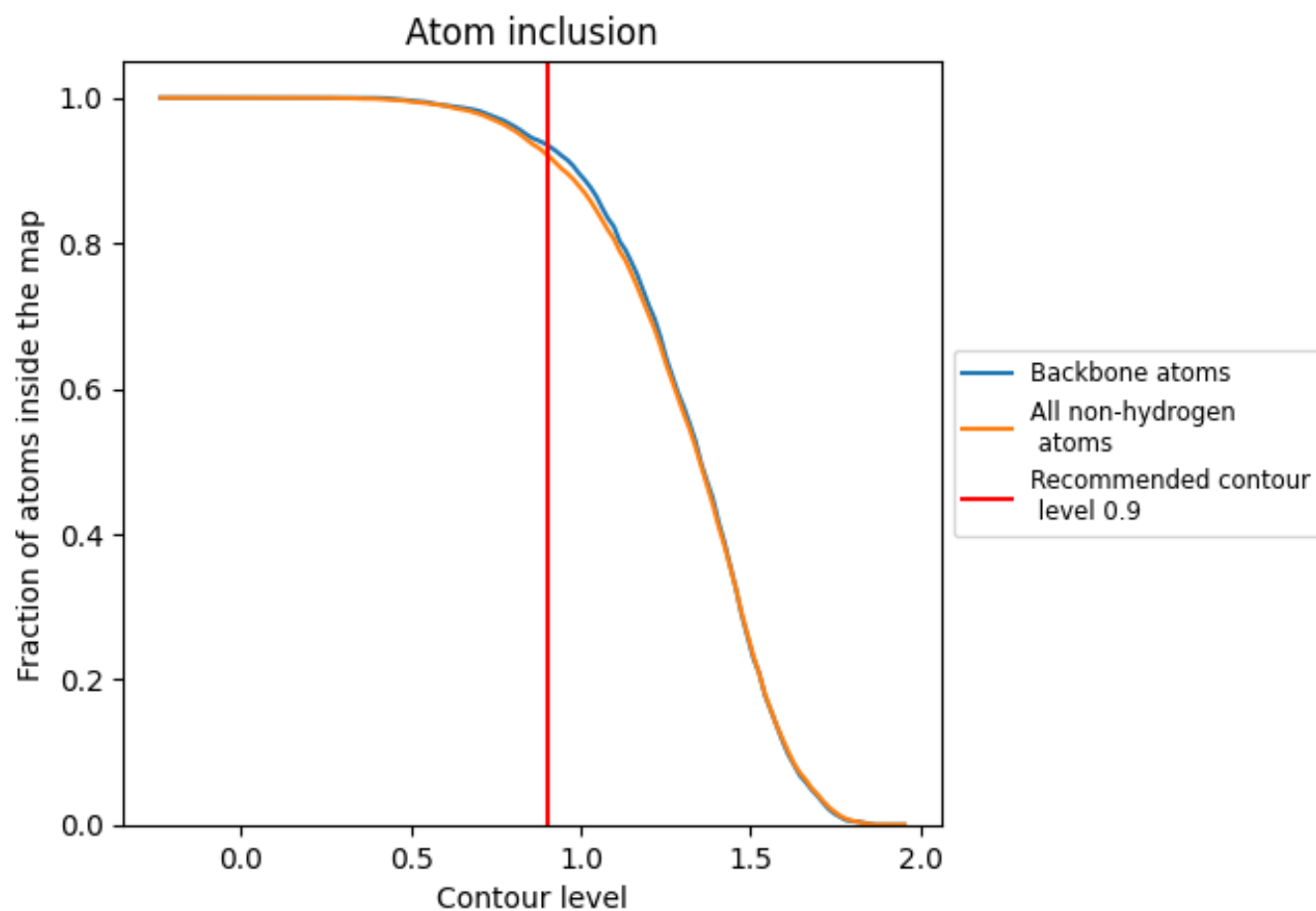
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.9).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9217	<div><div></div></div> 0.0380
A	<div><div></div></div> 0.9217	<div><div></div></div> 0.0380

