



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:10 AM UTC

PDB ID : 8FDU / pdb_00008fdu
EMDB ID : EMD-29014
Title : Engineered human dynein motor domain in the microtubule-unbound state with LIS1 complex in the buffer containing ATP-Vi (local refined on AAA3-AAA5 and LIS1)
Authors : Ton, W.; Wang, Y.; Chai, P.
Deposited on : 2022-12-04
Resolution : 3.30 Å (reported)

This is a wwPDB EM Validation Summary 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:

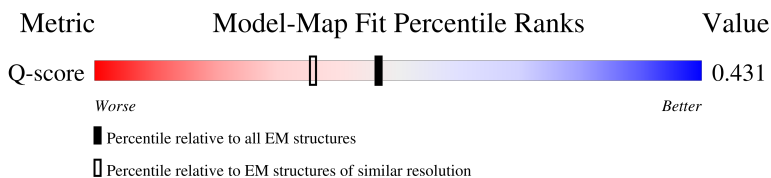
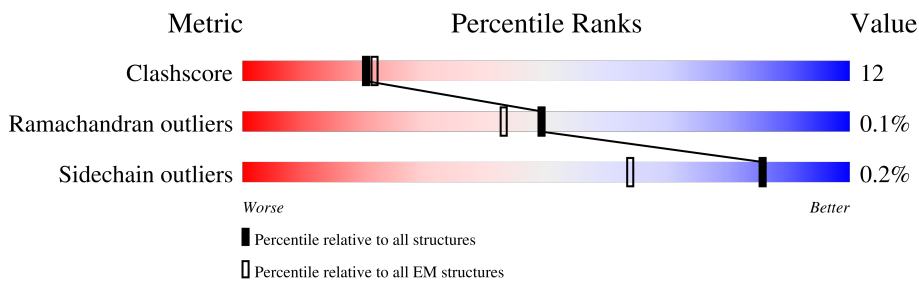
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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 $\leq 5\%$. 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	3126	<p>10% (upper red bar), 24% (red), 8% (orange), 68% (grey)</p>
2	B	598	<p>43% (red), 34% (orange), 19% (yellow), 47% (grey)</p>
2	C	598	<p>9% (upper red bar), 37% (red), 16% (yellow), 47% (grey)</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13193 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, Serine-tRNA ligase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1001	8141	5164	1425	1516	36	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q14204
A	2	SER	-	expression tag	UNP Q14204
A	3125	GLU	-	expression tag	UNP Q14204
A	3126	PHE	-	expression tag	UNP Q14204

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta, PI atelet-activating factor acetylhydrolase IB subunit beta, human LIS1 protein with a SNAP tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	316	2499	1571	441	467	20	0	0
2	C	316	2499	1571	441	467	20	0	0

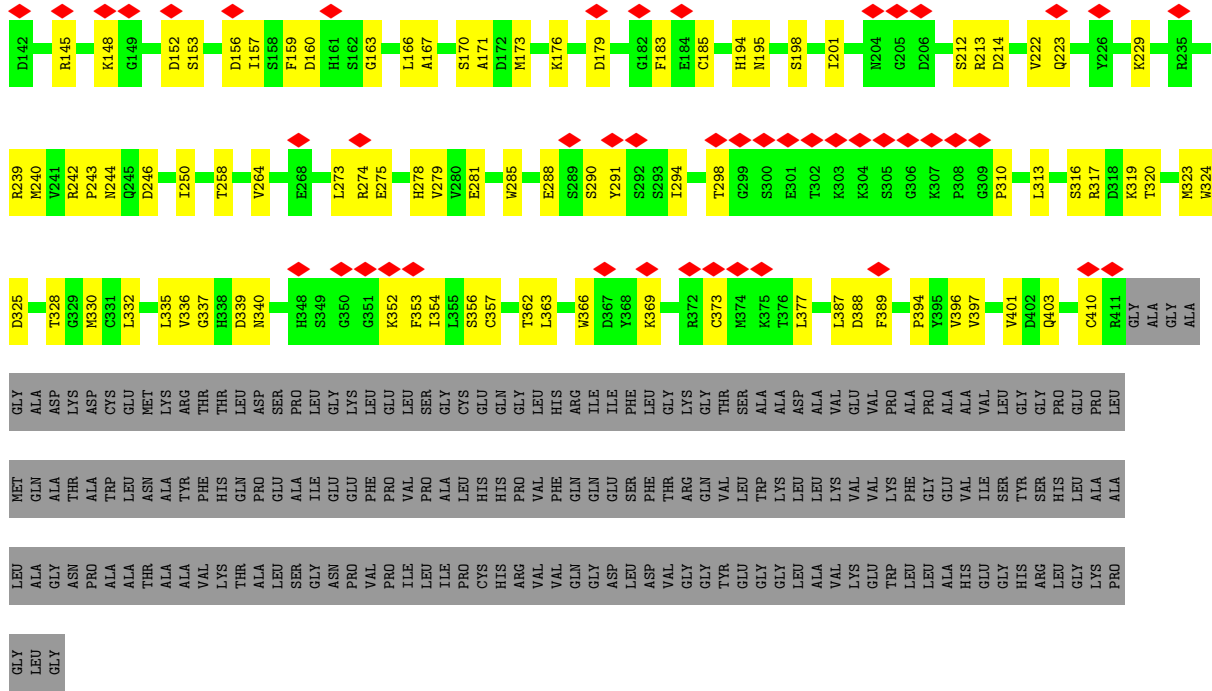
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P43034
B	2	SER	-	expression tag	UNP P43034
C	1	GLY	-	expression tag	UNP P43034
C	2	SER	-	expression tag	UNP P43034

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



GLN	VAL	GLN	ASP	R1155	Y1310	R1408	Y1512	E1594	E1686	L1763	LEU	LYS
LYS	SER	ARG	TYR	A1156	A1311	E1409	T1513	L1595	E1693	R1764	LEU	GLU
ARG	ARG	ALA	GLU	L1157	E1312	K1410	E1514	Y1596	V1694	R1765	ALA	ALA
GLN	CYS	ALA	VAL	P1158	P1313	A1411	E1515	K1597	F1694	R1765	ALA	ALA
TRP	GLY	TRP	ASP	D1159	M1316	M1412	D1516	W1598	V1695	ASP	GLN	GLN
ILE	MET	THR	ILE	M1160	M1318	S1413	F1517	F1599	H1696	ARG	GLU	GLU
VAL	VAL	TRP	SER	E1161	R1328	R1414	D1518	Q1602	Q1697	ILE	VAL	ALA
PHE	ASP	GLY	GLY	E1161	F1237	R1420	E1519	M1606	T1698	LYS	GLN	ARG
ASP	GLY	TRP	TRP	T1171	F1323	W1421	D1520	S1616	L1699	SER	GLN	GLN
GLY	SER	LEU	SER	T1172	Y1339	L1422	G1529	S1617	A1702	GLN	LEU	LEU
ASP	VAL	PRO	PRO	L1177	S1340	S1423	C1530	S1618	R1705	LEU	LYS	LYS
VAL	ASP	ARG	TRP	L1177	M1344	K1424	K1531	E1619	A1707	GLU	ARG	LYS
PRO	LEU	SER	GLN	D1181	T1345	D1425	M1532	G1618	L1706	VAL	LEU	VAL
ASN	GLY	THR	ILE	H1182	R1346	D1430	N1533	E1619	A1707	VAL	GLN	GLN
ASN	THR	GLN	THR	Y1183	W1347	Y1437	K1534	L1620	K1708	ALA	ALA	ALA
ASN	THR	GLN	THR	C1184	V1348	V1438	T1538	L1622	R1709	ALA	ALA	ALA
ASN	THR	GLN	THR	E1101	R1349	V1438	M1539	D1622	G1710	ALA	THR	LYS
ASN	THR	GLN	THR	V1102	F1352	V1438	D1540	R1623	G1711	ASN	GLU	ASP
ASN	THR	GLN	THR	E1103	E1353	R1441	E1541	A1624	R1712	ASP	ARG	ASN
VAL	PHE	VAL	ILE	Y1186	E1353	L1456	E1542	A1625	T1713	LYS	ASN	GLN
VAL	LEU	VAL	ILE	R1187	E1353	H1463	M1543	T1626	M1714	LYS	GLN	GLN
VAL	LEU	VAL	ILE	R1188	R1356	I1467	V1544	L1630	A1715	LYS	VAL	VAL
VAL	LEU	VAL	ILE	R1189	P1357	D1451	V1544	F1631	H1720	LYS	ALA	ALA
VAL	LEU	VAL	ILE	P1190	L1358	L1456	D1546	M1632	Y1721	LYS	ARG	ASN
VAL	LEU	VAL	ILE	M1191	E1359	L1456	S1547	N1632	Y1721	VAL	ARG	ASN
VAL	LEU	VAL	ILE	G1192	T1360	H1463	G1548	R1633	Y1728	VAL	ARG	ASN
VAL	LEU	VAL	ILE	V1193	F1362	I1467	F1549	V1635	Y1732	VAL	ARG	ASN
VAL	LEU	VAL	ILE	V1194	Y1363	I1467	L1550	M1637	F1732	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	L1366	I1470	E1551	D1641	H1733	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1367	F1471	E1552	W1642	E1734	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	L1368	R1472	M1553	M1642	K1735	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	W1370	L1478	L1556	E1645	R1736	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	L1368	L1478	L1556	E1645	S1737	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	A1371	L1479	E1561	E1645	E1738	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	A1374	L1480	E1561	E1645	L1739	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	Q1379	L1481	G1568	K1657	E1740	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	D1380	L1482	D1569	M1658	E1741	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	R1381	G1483	E1570	L1660	Q1742	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	D1382	S1484	E1570	L1660	Q1743	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	D1382	G1485	E1570	L1660	M1744	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	D1382	K1488	T1576	I1666	H1745	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	E1386	K1488	Q1577	D1669	L1746	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	R1388	M1498	C1578	D1669	M1747	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	R1389	M1498	K1579	Y1670	V1748	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	D1392	L1501	E1580	M1671	G1749	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	S1502	A1582	M1671	L1750	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	V1503	Q1583	V1672	L1751	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	V1504	Q1583	V1672	K1752	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	Q1505	K1584	Y1675	L1753	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	I1506	K1584	D1676	L1754	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	I1507	E1586	K1677	K1754	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	V1508	G1586	L1678	E1755	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	H1509	L1587	P1679	T1756	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	R1510	M1588	Q1680	V1757	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	K1511	L1589	P1681	D1758	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	R1511	L1589	P1682	Q1759	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	R1511	L1589	S1683	V1760	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	R1511	L1589	S1683	E1762	VAL	ARG	ASN
VAL	LEU	VAL	ILE	L1195	I1395	R1511	L1589	S1683	E1762	VAL	ARG	ASN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53572	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.105	Depositor
Minimum map value	-0.506	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	413.64, 413.64, 413.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.149, 1.149, 1.149	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

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	0/8319	0.50	1/11279 (0.0%)
2	B	0.33	1/2563 (0.0%)	0.51	1/3472 (0.0%)
2	C	0.32	0/2563	0.49	1/3472 (0.0%)
All	All	0.33	1/13445 (0.0%)	0.50	3/18223 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	ARG	N-CA	5.07	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1674	VAL	N-CA-C	-6.46	106.52	111.62
2	C	99	PRO	N-CA-C	6.33	118.42	110.70
2	B	99	PRO	N-CA-C	5.60	117.54	110.70

There are no chirality outliers.

There are no planarity outliers.

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	8141	0	8095	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2499	0	2434	84	0
2	C	2499	0	2434	65	0
3	A	54	0	24	4	0
All	All	13193	0	12987	319	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.

The worst 5 of 319 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:1142:PRO:HD3	1:A:1258:ASN:ND2	1.84	0.92
1:A:1142:PRO:HD3	1:A:1258:ASN:HD21	1.36	0.91
1:A:1292:ILE:HD13	3:A:3201:ADP:N6	1.89	0.87
1:A:2256:ALA:HB1	1:A:2260:ARG:HH12	1.37	0.86
1:A:1745:HIS:ND1	1:A:2232:ASN:ND2	2.27	0.83

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	997/3126 (32%)	959 (96%)	38 (4%)	0	100	100
2	B	314/598 (52%)	298 (95%)	16 (5%)	0	100	100
2	C	314/598 (52%)	301 (96%)	12 (4%)	1 (0%)	36	65
All	All	1625/4322 (38%)	1558 (96%)	66 (4%)	1 (0%)	49	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	107	GLY

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	901/2766 (33%)	900 (100%)	1 (0%)	88	90
2	B	281/505 (56%)	280 (100%)	1 (0%)	84	84
2	C	281/505 (56%)	280 (100%)	1 (0%)	84	84
All	All	1463/3776 (39%)	1460 (100%)	3 (0%)	85	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1503	VAL
2	B	120	VAL
2	C	109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2232	ASN
2	B	181	GLN
2	C	155	GLN
2	B	192	HIS
1	A	1697	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	3201	-	28,29,29	0.46	0	43,45,45	0.51	0
3	ADP	A	3202	-	28,29,29	0.49	0	43,45,45	0.50	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
3	ADP	A	3201	-	-	1/16/32/32	0/3/3/3
3	ADP	A	3202	-	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3201	ADP	PA-O3A-PB-O3B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

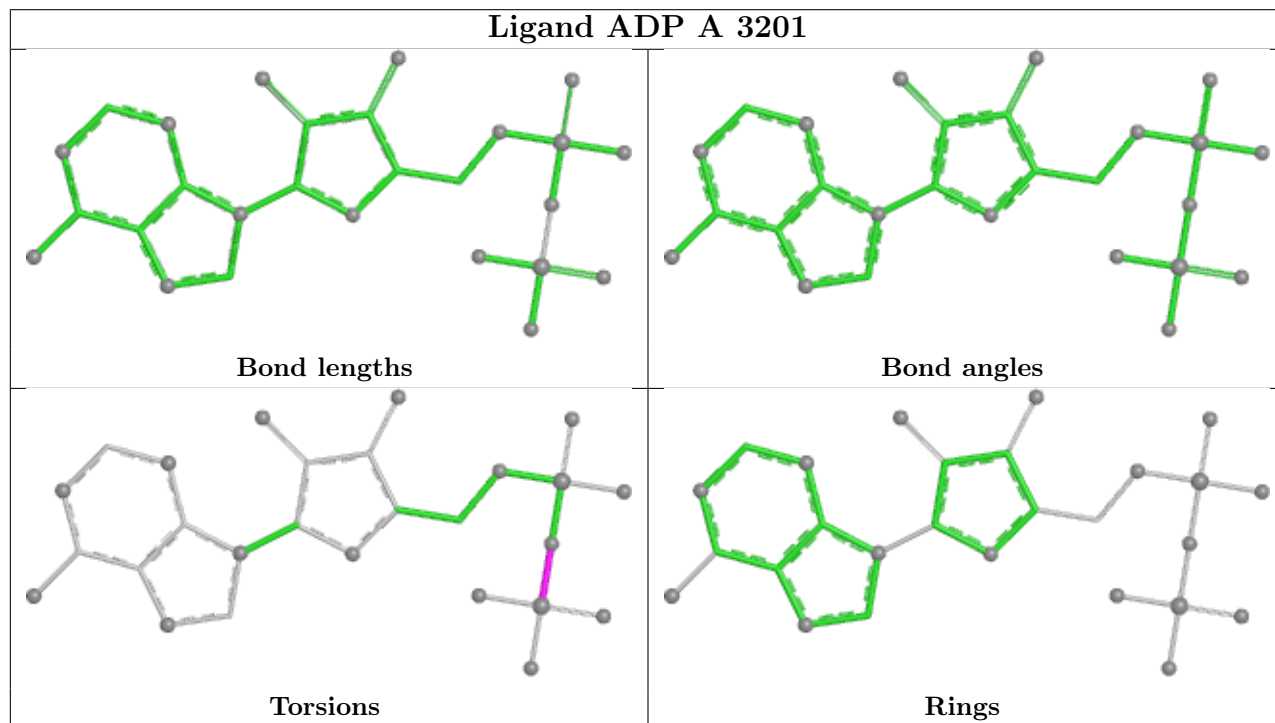
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3201	ADP	3	0

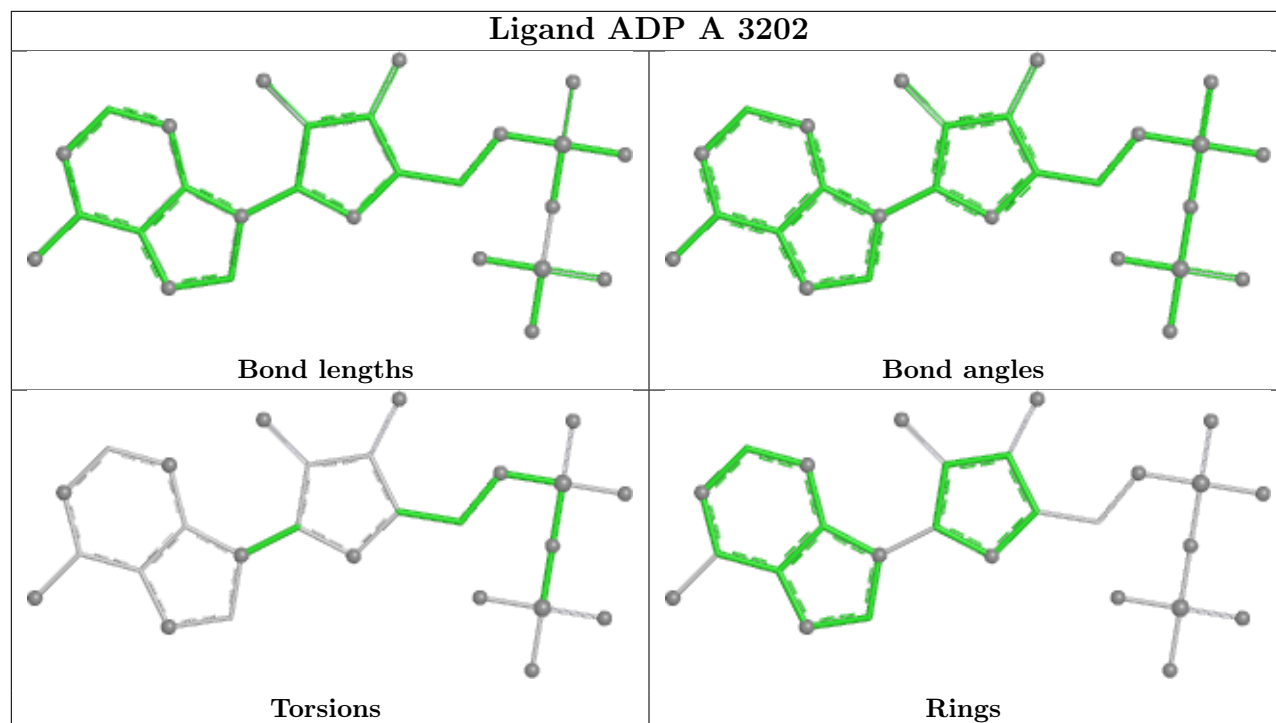
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3202	ADP	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

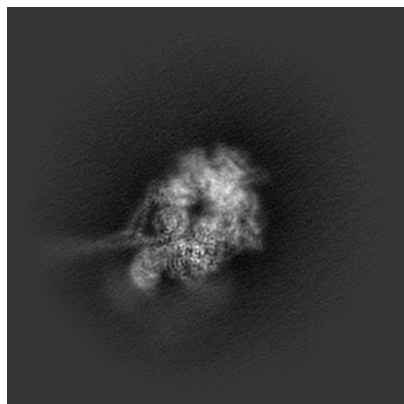
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29014. These allow visual inspection of the internal detail of the map and identification of artifacts.

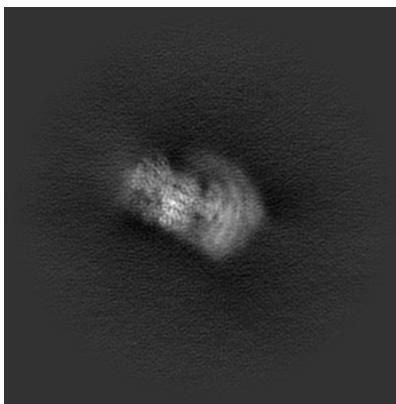
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

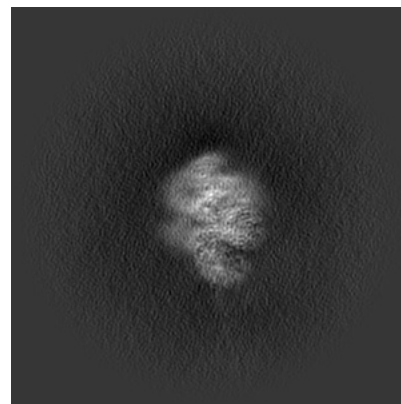
6.1.1 Primary map



X

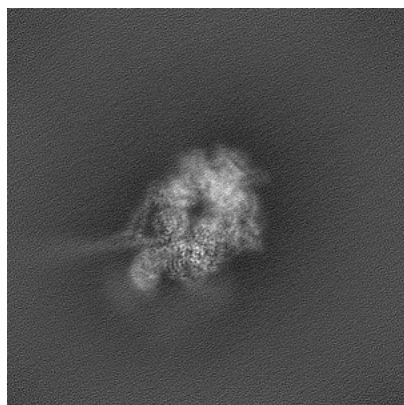


Y

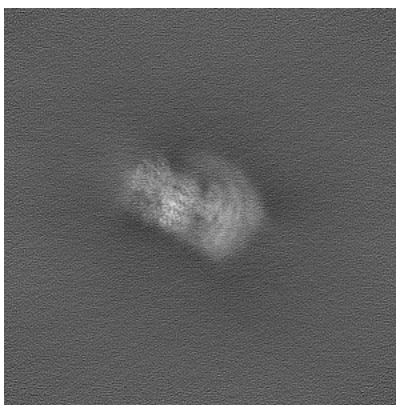


Z

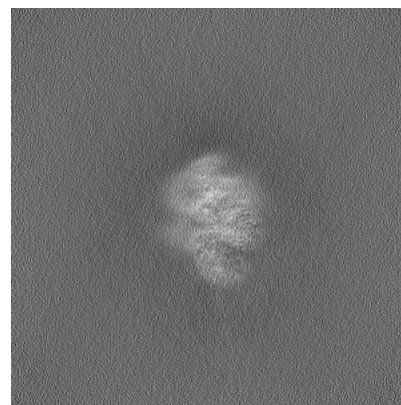
6.1.2 Raw map



X



Y

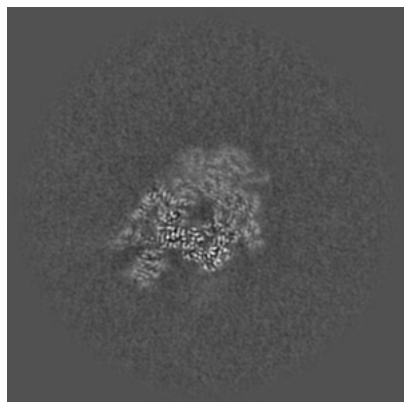


Z

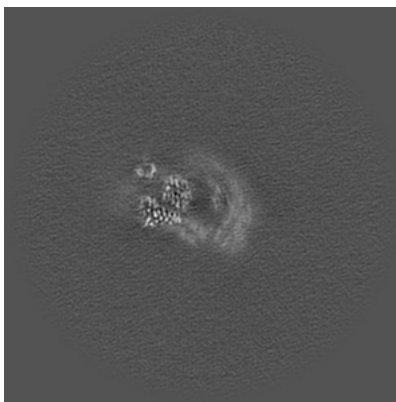
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

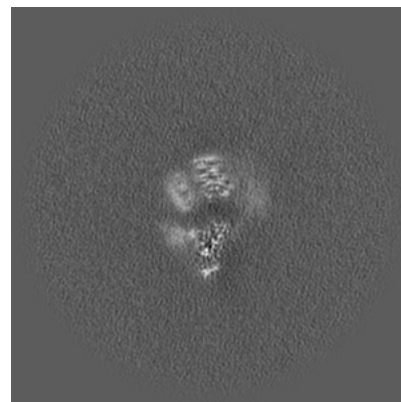
6.2.1 Primary map



X Index: 180

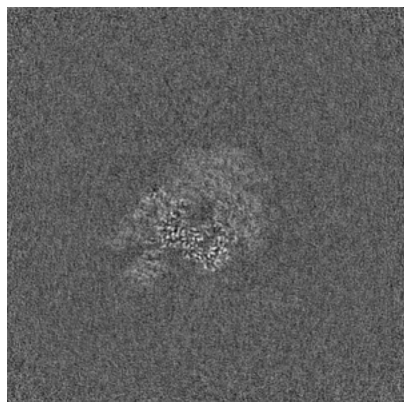


Y Index: 180

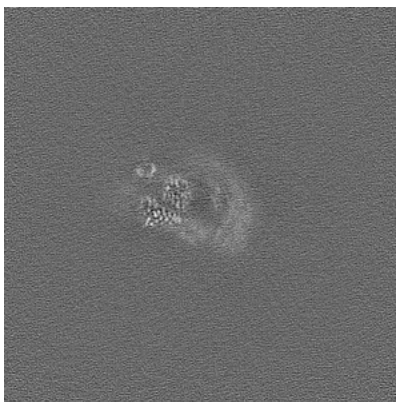


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180

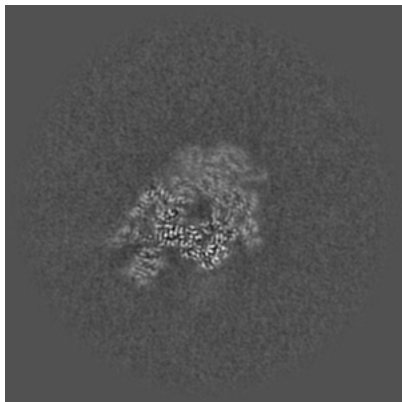


Z Index: 180

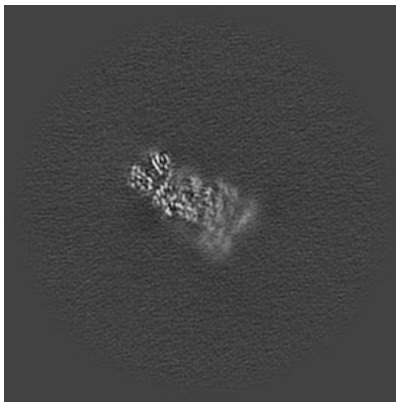
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

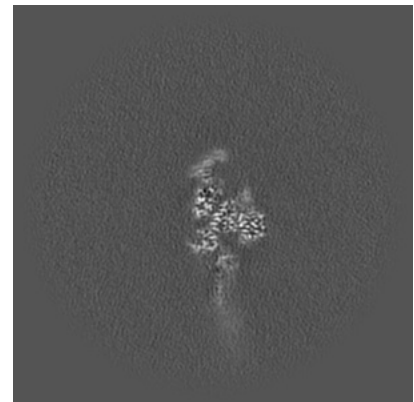
6.3.1 Primary map



X Index: 180

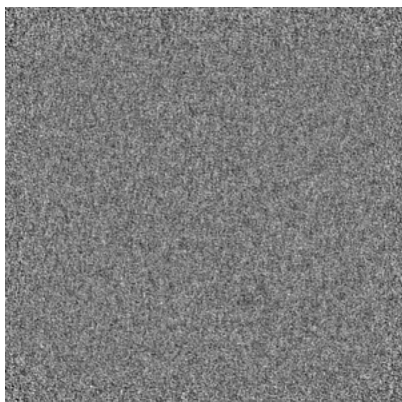


Y Index: 158

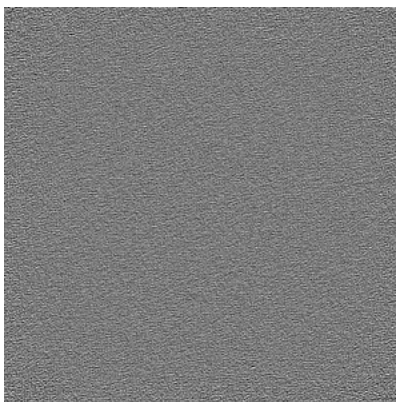


Z Index: 144

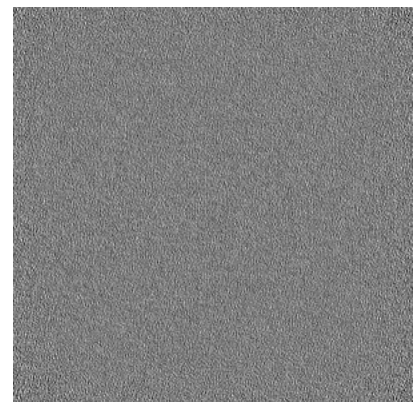
6.3.2 Raw map



X Index: 0



Y Index: 0

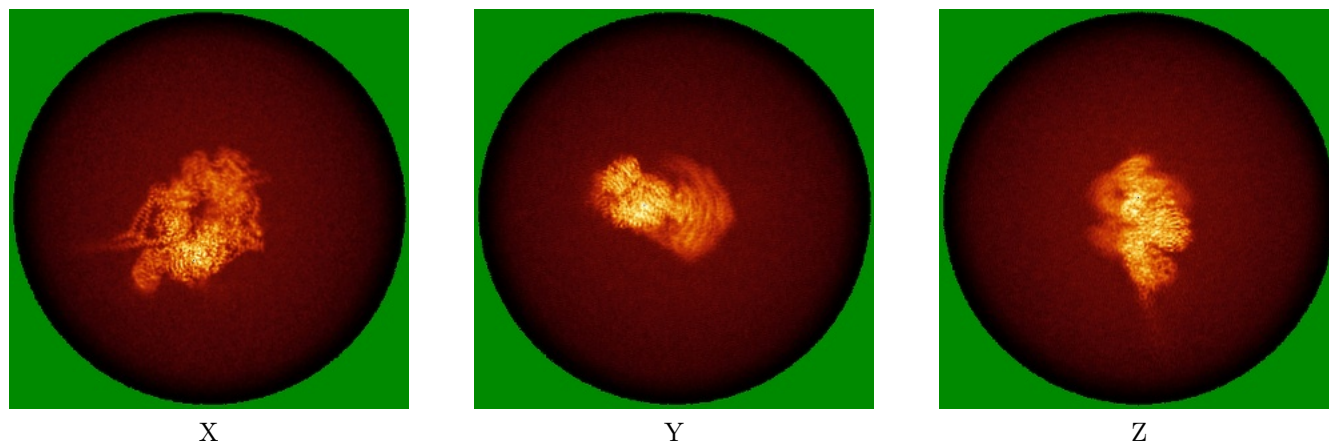


Z Index: 0

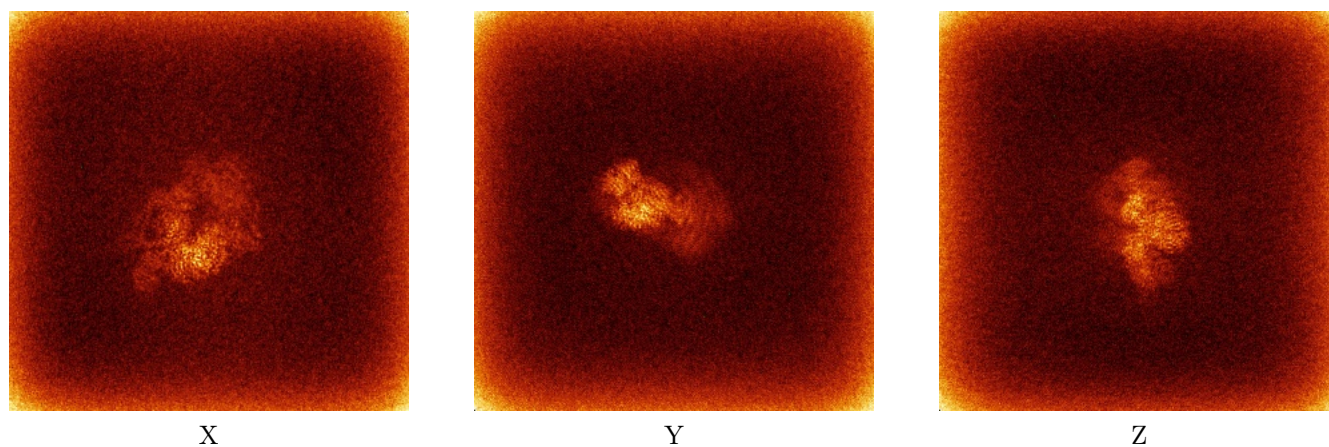
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



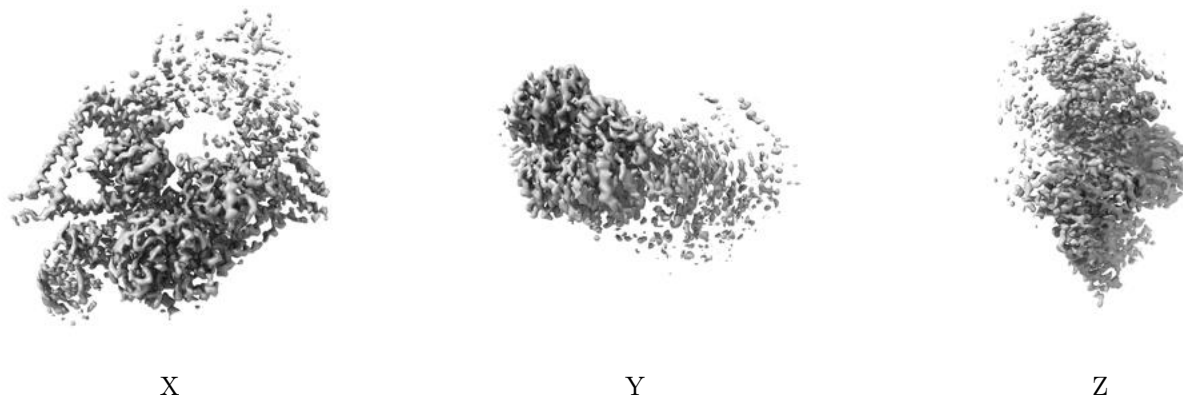
6.4.2 Raw map



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



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.

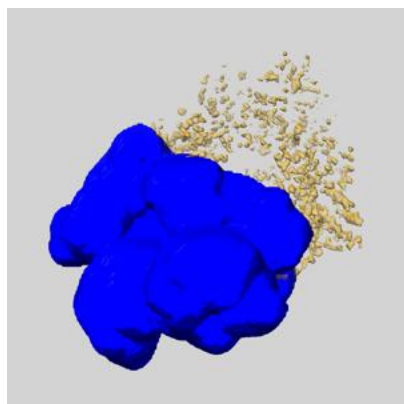
6.6 Mask visualisation [i](#)

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

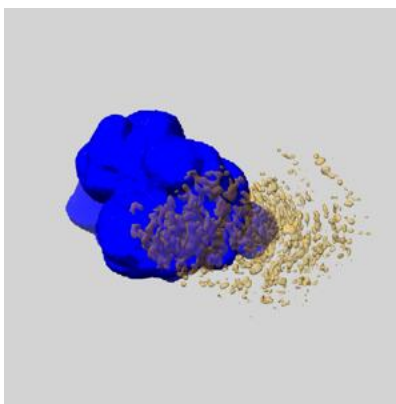
A mask typically either:

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

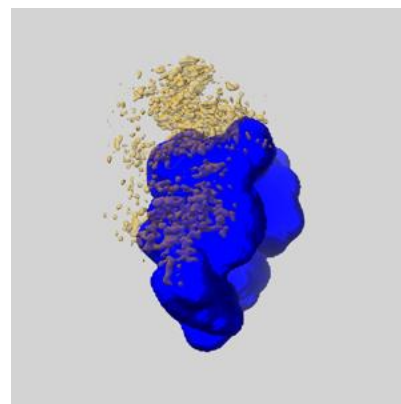
6.6.1 emd_29014_msk_1.map [i](#)



X



Y

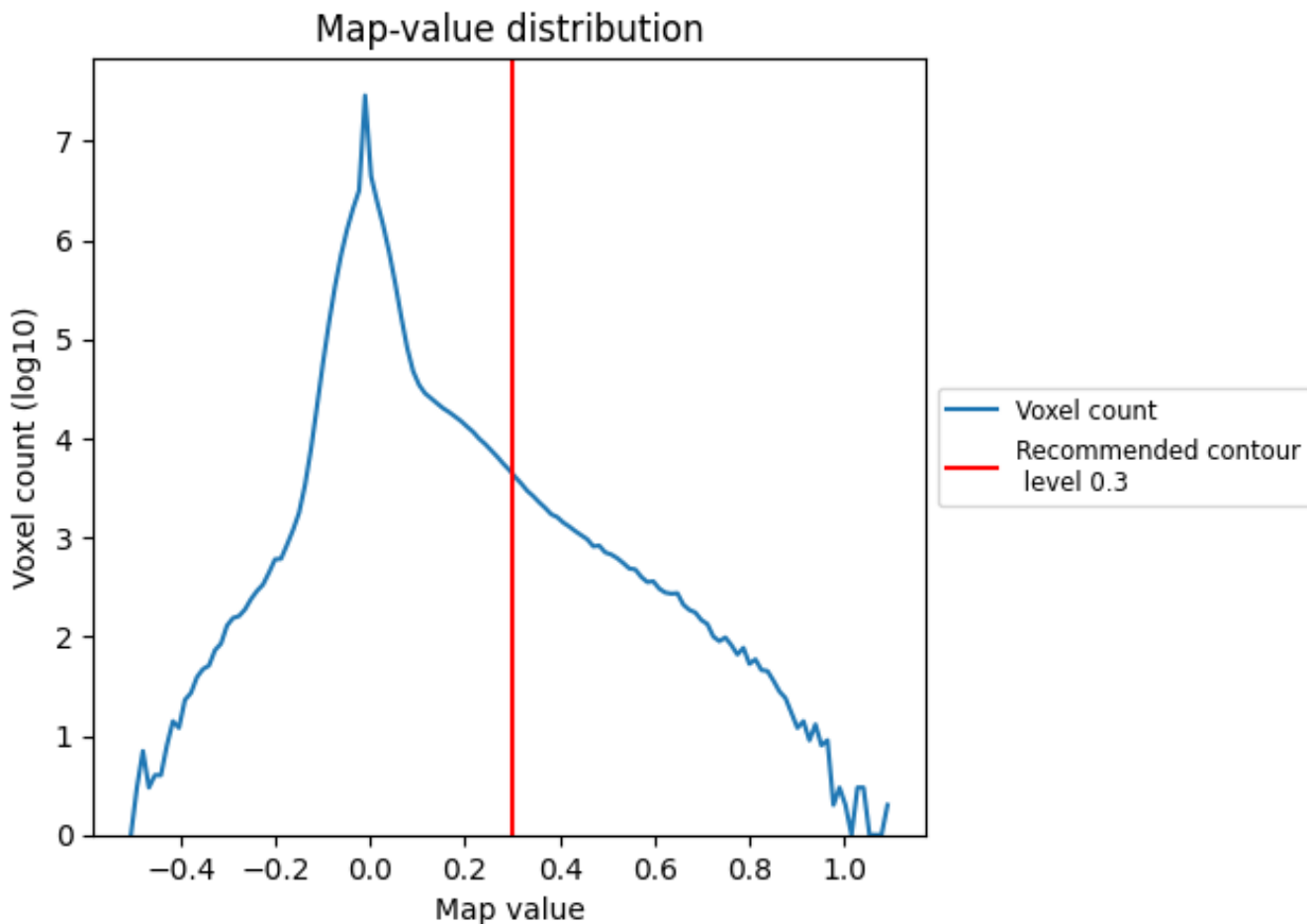


Z

7 Map analysis [i](#)

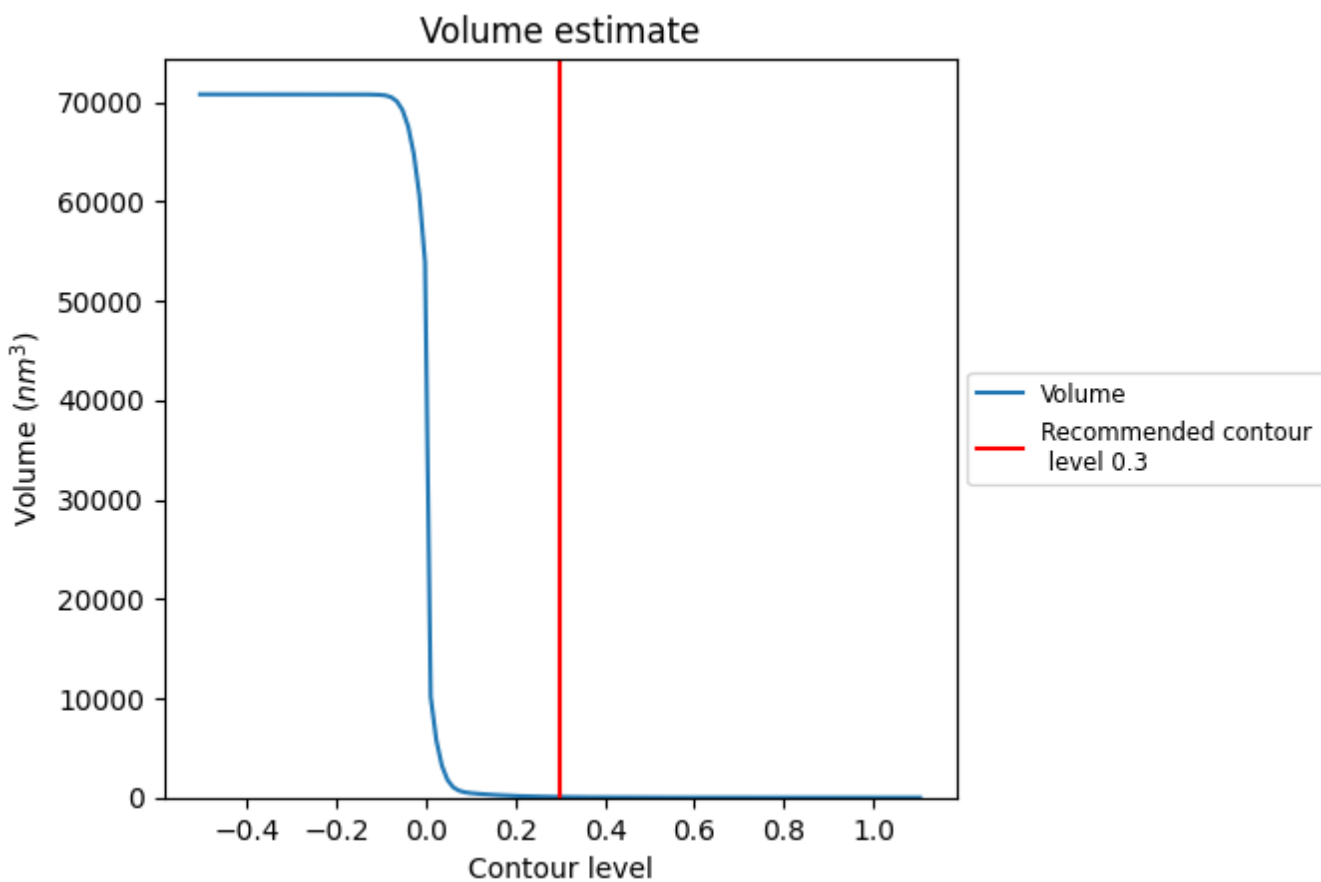
This section contains the results of statistical analysis of the map.

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.

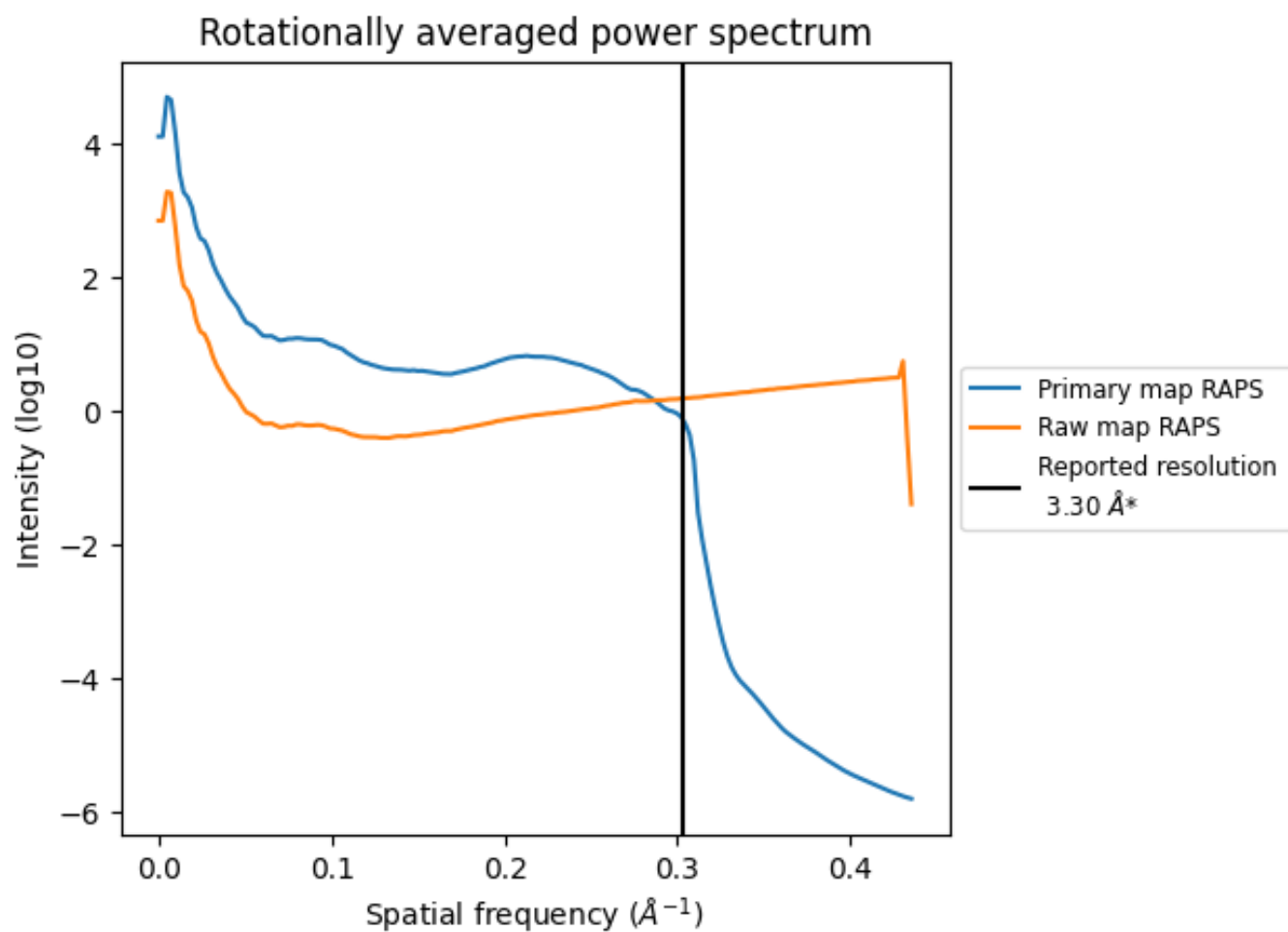
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 58 nm³; this corresponds to an approximate mass of 52 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

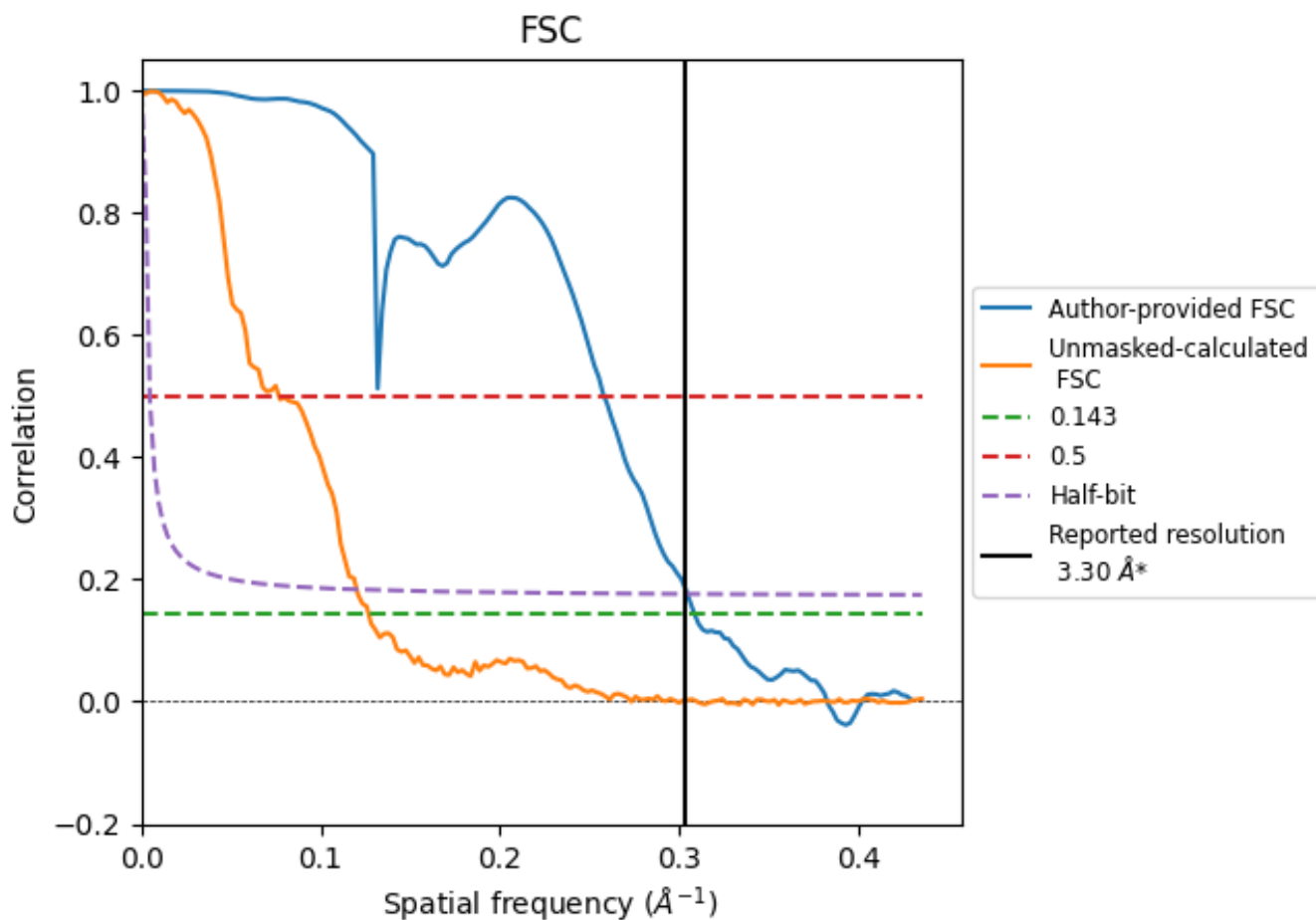


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

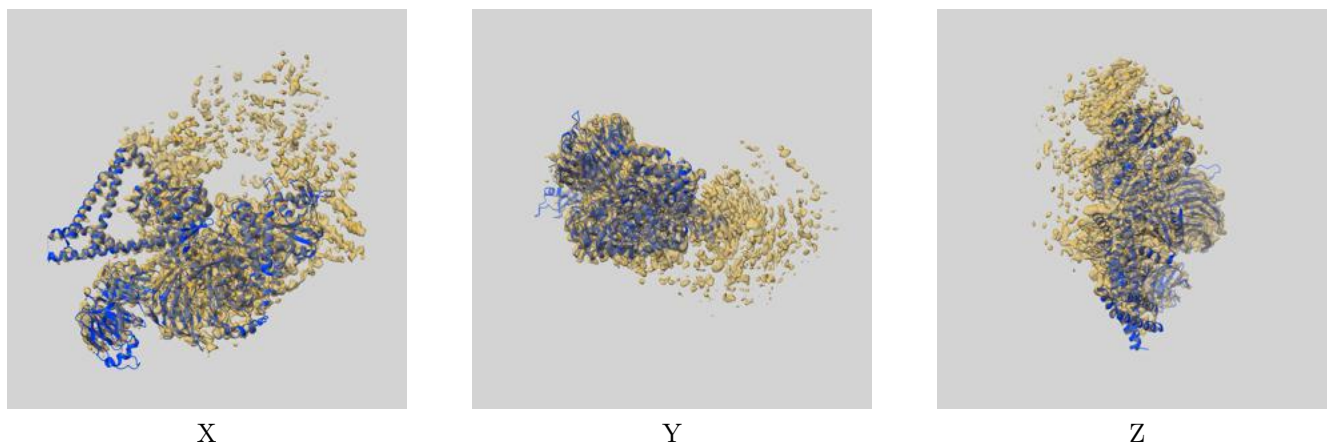
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.24	3.88	3.29
Unmasked-calculated*	7.89	13.02	8.33

*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 7.89 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

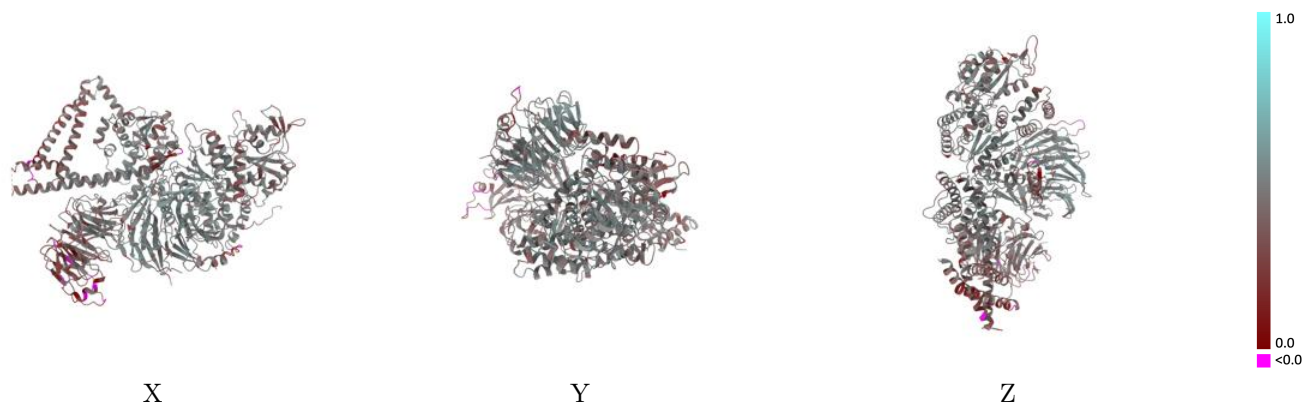
This section contains information regarding the fit between EMDB map EMD-29014 and PDB model 8FDU. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



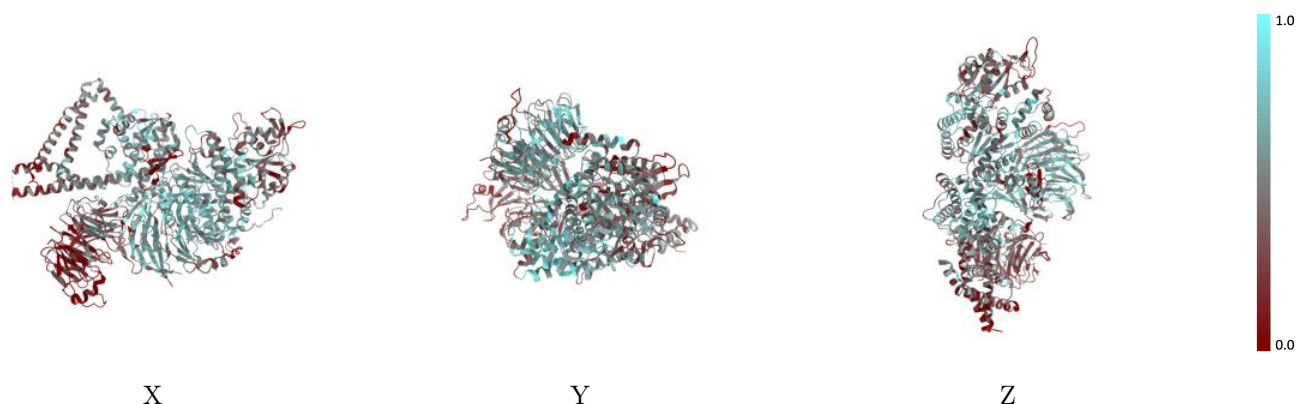
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



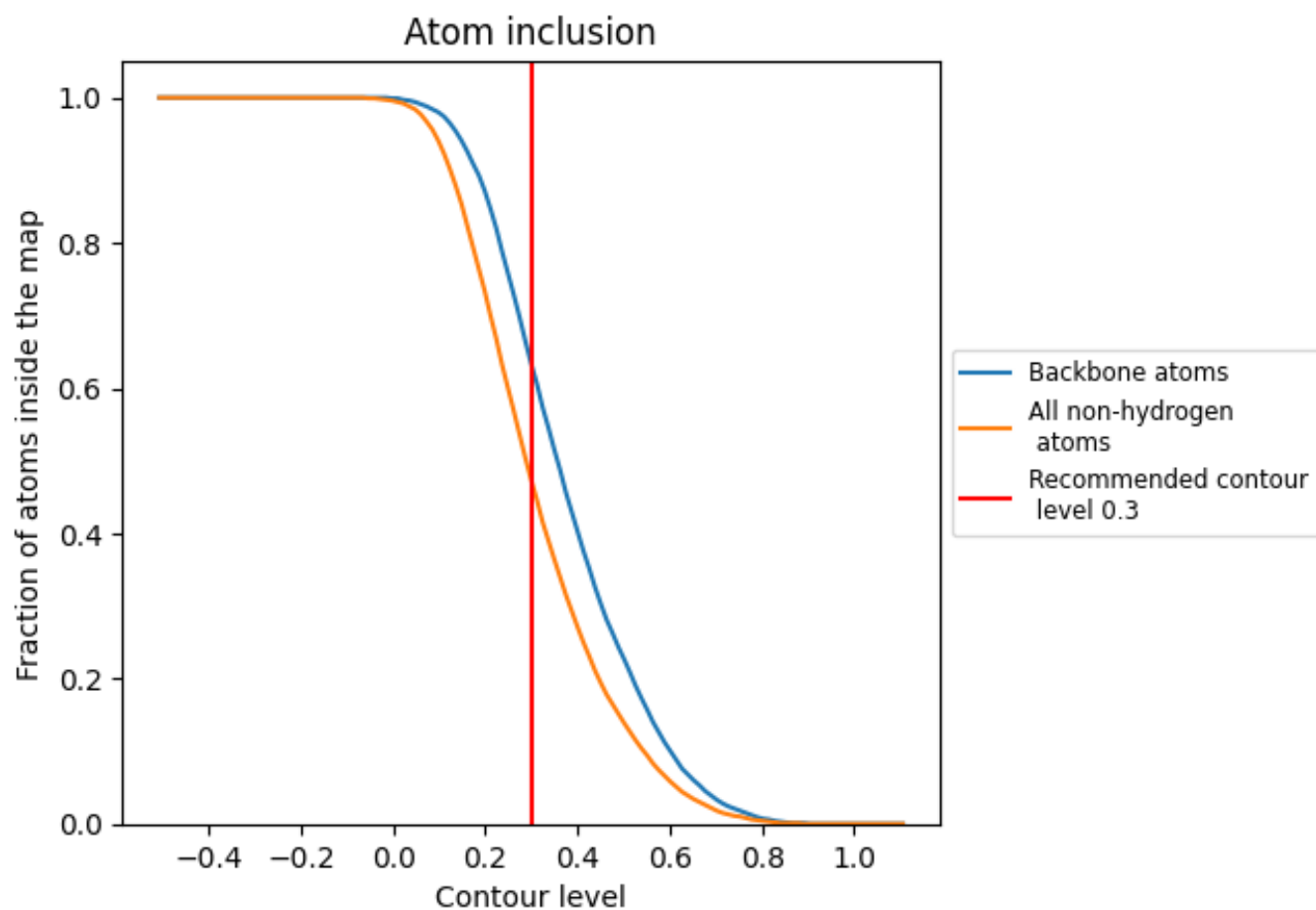
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 47% 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	■ 0.4730	■ 0.4310
A	■ 0.5180	■ 0.4410
B	■ 0.2050	■ 0.3470
C	■ 0.5930	■ 0.4830

