



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 10:47 PM JST

PDB ID : 7CPX
EMDB ID : EMD-30434
Title : Lovastatin nonaketide synthase
Authors : Wang, J.; Wang, Z.
Deposited on : 2020-08-08
Resolution : 2.91 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.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) : 2.31.3

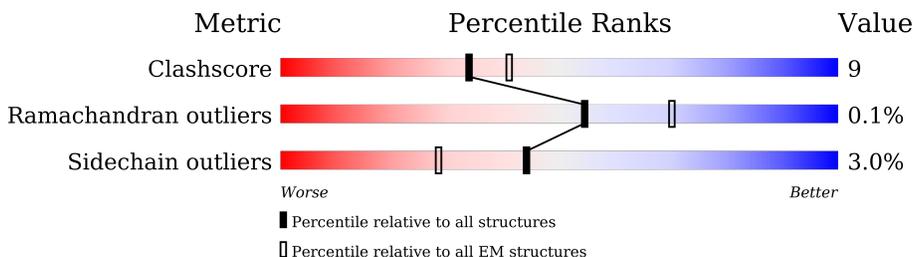
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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 ≥ 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	3046	
1	B	3046	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 70118 atoms, of which 34718 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.

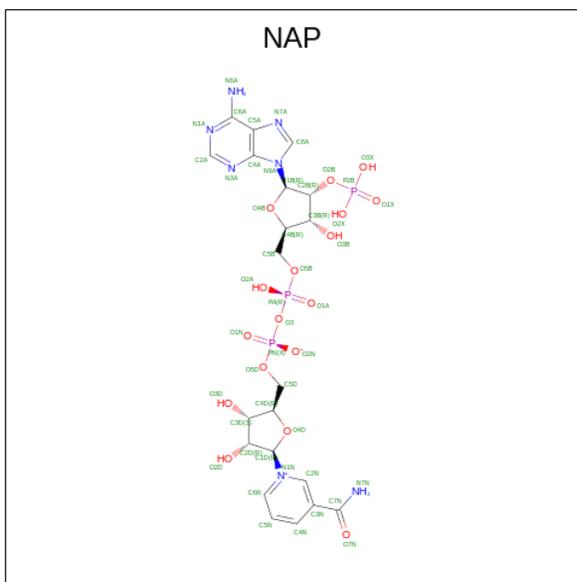
- Molecule 1 is a protein called Lovastatin nonaketide synthase, polyketide synthase component.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2262	Total	C	H	N	O	S	0	0
			34986	11177	17334	3061	3325	89		
1	B	2262	Total	C	H	N	O	S	0	0
			34986	11177	17334	3061	3325	89		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1884	GLN	GLY	engineered mutation	UNP Q9Y8A5
A	1885	ALA	GLN	engineered mutation	UNP Q9Y8A5
A	3039	HIS	-	expression tag	UNP Q9Y8A5
A	3040	VAL	-	expression tag	UNP Q9Y8A5
A	3041	HIS	-	expression tag	UNP Q9Y8A5
A	3042	HIS	-	expression tag	UNP Q9Y8A5
A	3043	HIS	-	expression tag	UNP Q9Y8A5
A	3044	HIS	-	expression tag	UNP Q9Y8A5
A	3045	HIS	-	expression tag	UNP Q9Y8A5
A	3046	HIS	-	expression tag	UNP Q9Y8A5
B	1884	GLN	GLY	engineered mutation	UNP Q9Y8A5
B	1885	ALA	GLN	engineered mutation	UNP Q9Y8A5
B	3039	HIS	-	expression tag	UNP Q9Y8A5
B	3040	VAL	-	expression tag	UNP Q9Y8A5
B	3041	HIS	-	expression tag	UNP Q9Y8A5
B	3042	HIS	-	expression tag	UNP Q9Y8A5
B	3043	HIS	-	expression tag	UNP Q9Y8A5
B	3044	HIS	-	expression tag	UNP Q9Y8A5
B	3045	HIS	-	expression tag	UNP Q9Y8A5
B	3046	HIS	-	expression tag	UNP Q9Y8A5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).

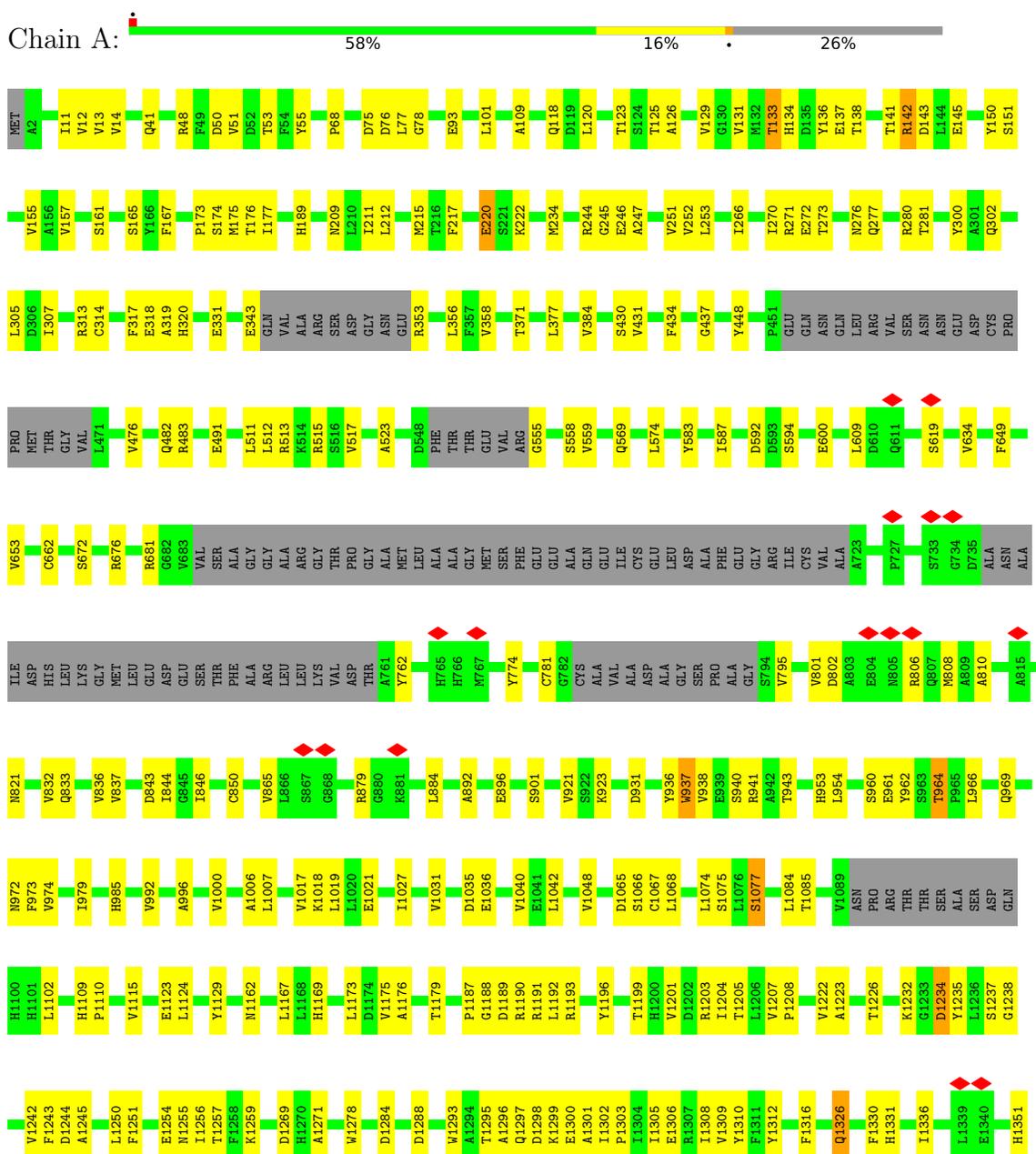


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	A	1	Total	C	H	N	O	P	0
			73	21	25	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			73	21	25	7	17	3	

3 Residue-property plots

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.

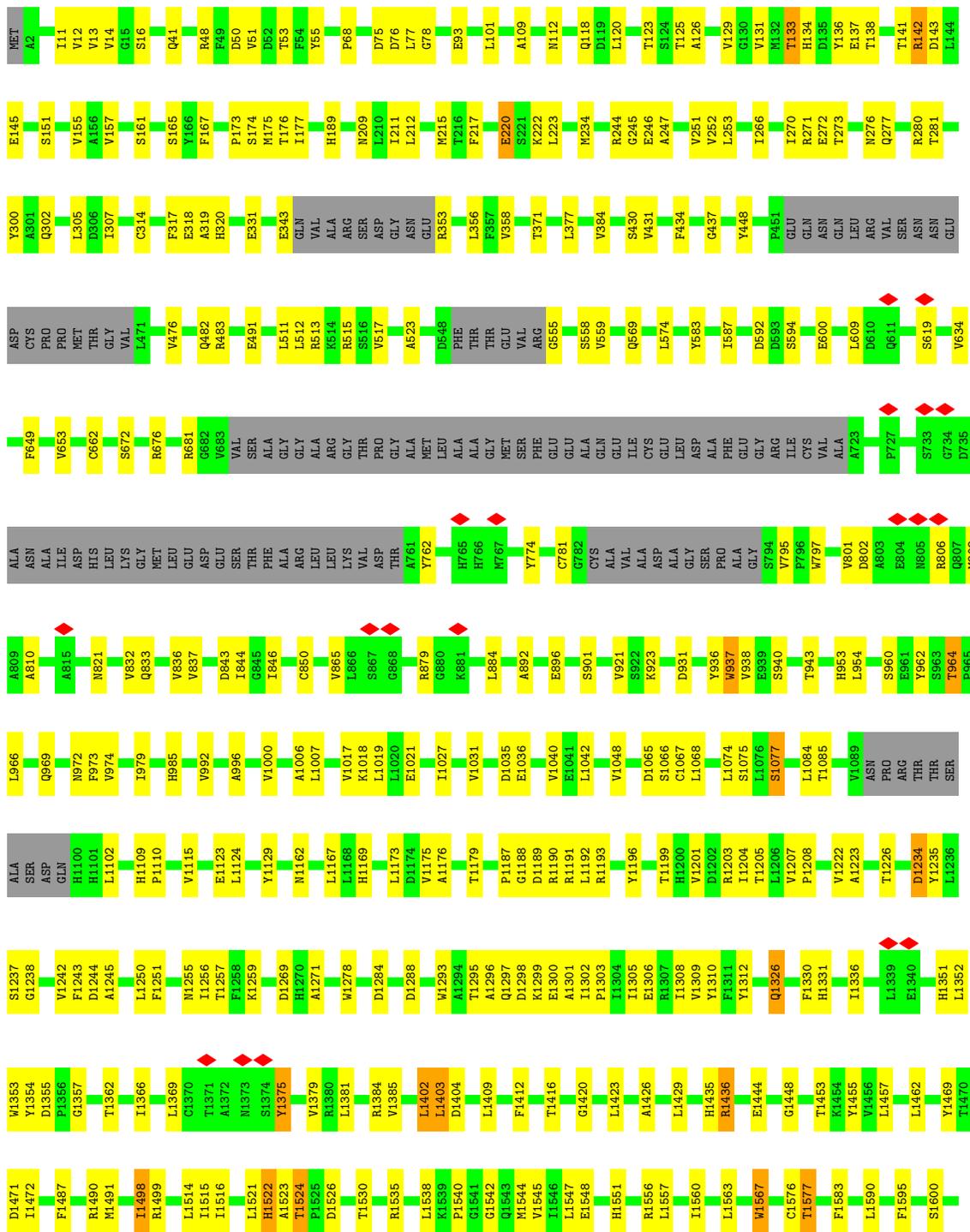
- Molecule 1: Lovastatin nonaketide synthase, polyketide synthase component



ALA THR ARG GLU THR PRO TYR VAL VAL GLU MET ASP ASP THR LYS ASP PRO PRO LEU LEU THR ALA LYS LEU LEU GLN SER SER ARG TYR ALA ALA HIS HIS PRO ALA PHE LEU GLU SER TYR MET SER MET MET ASN PRO ALA LEU LYS LEU

ALA HIS VAL HIS HIS HIS HIS HIS HIS

● Molecule 1: Lovastatin nonaketide synthase, polyketide synthase component



TI603	D1604	R1605	L1609	P1610	P1611	TI612	S1613	V1614	F1615	S1616	TI617	D1621	A1622	TI623	V1624	E1625	V1626	LEU	ASP	ALA	PRO	LEU	ALA	LEU	SER	GLY	THR	VAL	LYS	ASP	SER	Y1641	P1642	V1646	TI651	Q1655	R1656	L1657	L1658	E1683	F1691	E1700	L1701	F1702	L1705	TI706	K1714	TI723
V1724	W1725	L1726	W1731	V1732	W1733	A1738	S1739	TI740	L1744	R1745	S1746	R1747	R1748	R1749	L1759	D1760	TI766	PHE	ASP	ALA	THR	PHE	LEU	V1773	L1777	E1780	E1781	TI790	TI791	W1792	TI793	Q1794	E1797	W1800	R1804	TI807	P1808	R1809	R1812	D1813	R1816	R1824	M1830					
L1840	R1844	TI856	V1859	V1863	Q1864	Q1865	M1866	C1877	V1883	Q1884	F1888	R1911	R1919	A1927	L1938	M1939	V1940	TI941	V1942	L1943	L1948	V1952	TI953	S1954	THR	ALA	LYS	CYS	LEU	V1961	TI962	D1963	M1969	P1970	P1971	C1974	G1975	A1992	S1995	GLY	ASN							
ARG	SER	SER	SER	SER	ALA	GLY	ASP	S2008	R2015	Q2030	D2034	A2061	T2066	S2070	THR	GLU	LEU	HIS	GLY	SER	ARG	HIS	GLN	ALA	L2083	Y2087	W2088	E2089	H2090	L2094	A2095	R2096	L2099	E2104	V2108	C2111	S2126	T2127	I2129	I2147								
D2148	A2149	E2150	T2158	D2167	L2168	G2169	R2170	R2174	W2175	R2176	V2177	Q2178	H2179	C2182	T2187	R2196	R2207	P2234	G2237	F2241	G2242	F2243	V2245	M2250	L2251	M2252	M2253	M2254	E2255	L2256	M2261	V2262	L2263	V2267	V2270	H2274	S2278	D2287	F2288	F2289								
I2295	V2296	A2297	G2300	N2311	C2312	L2314	Q2315	A2316	Q2319	Q2320	R2321	V2322	T2330	I2331	D2332	R2355	D2359	S2360	V2361	E2362	E2365	T2368	A2371	E2372	V2375	Q2387	V2383	L2394	D2395	N2396	L2399	E2400	L2401	T2403	G2404	P2422	R2423	N2426	L2427	K2428	E2431							
Y2432	ARG	GLY	ALA	LYS	ALA	GLY	GLY	LYS	Q2319	Q2320	R2321	V2322	T2330	I2331	D2332	R2355	D2359	S2360	V2361	E2362	E2365	T2368	A2371	E2372	V2375	Q2387	V2383	L2394	D2395	N2396	L2399	E2400	L2401	T2403	G2404	P2422	R2423	N2426	L2427	K2428	E2431							
ILE	ASP	GLN	GLY	VAL	ASP	SER	LEU	GLY	THR	THR	TRP	PHE	GLY	LYS	GLN	THR	ASN	LEU	LEU	ASP	GLN	VAL	ARG	GLY	ILE	VAL	ASP	ILE	ASP	THR	ASP	LEU	ALA	THR	GLY	LEU	ILE	PRO	PRO	VAL	VAL	THR	THR	TRP				
GLY	ALA	GLU	THR	ASP	ASN	THR	THR	GLY	GLY	ARG	GLU	ASP	THR	LYS	GLN	LEU	TRP																															
ARG	ILE	GLN	GLY	GLY	ALA	GLU	ASP	ASN	THR	THR	ILE	GLY	MET	PHE	MET	GLY	LEU	PHE																														
GLY	GLN	THR	LYS	VAL	VAL	GLN	ASP	ASP	ASN	THR	ALA	GLY	GLY	GLY	GLY	TYR	ARG	GLN	VAL																													
GLY	ASP	GLY	THR	THR	GLU	ASN	THR	GLY	GLN	GLN	TYR	ASP	THR	THR	THR	SER	PRO	HIS	VAL	SER																												
SER	ILE	PRO	VAL	LEU	PRO	LEU	MET	LEU	THR	SER	THR	ASP	THR	THR	THR	ASP	PHE	GLN	GLN	HIS	CYS	PRO	GLY	PRO	ASP	THR	PHE																					
TYR	LEU	ALA	ARG	TYR	GLN	VAL	VAL	LEU	ASP	SER	THR	THR	VAL	VAL	VAL	GLY	PRO	ARG	ALA	ALA	ASN	GLN	VAL	LEU																								
ILE	ALA	THR	ARG	GLU	ALA	ALA	ARG	THR	THR	VAL	THR	TYR	VAL																																			
LYS	ILE	THR	GLU	VAL	ILE	ALA	THR	MET																																								
ASN	PRO	ALA	LEU	LYS	LEU	ALA	HIS	MET																																								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	205047	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0075	Depositor
Map size (\AA)	350.0, 350.0, 350.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	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: NAP

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	0.25	0/18071	0.49	0/24587
1	B	0.25	0/18071	0.49	0/24587
All	All	0.25	0/36142	0.49	0/49174

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	17652	17334	17276	319	0
1	B	17652	17334	17276	320	0
2	A	48	25	25	0	0
2	B	48	25	25	0	0
All	All	35400	34718	34602	630	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 9.

The worst 5 of 630 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:B:1234:ASP:OD1	1:B:1844:ARG:NH1	2.12	0.82
1:A:1234:ASP:OD1	1:A:1844:ARG:NH1	2.12	0.82
1:B:1176:ALA:O	1:B:1179:THR:OG1	2.01	0.78
1:A:2315:GLN:NE2	1:A:2332:ASP:OD2	2.17	0.78
1:A:2431:GLU:OE1	1:A:2432:TYR:N	2.17	0.78

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	2236/3046 (73%)	2121 (95%)	113 (5%)	2 (0%)	51	81
1	B	2236/3046 (73%)	2121 (95%)	113 (5%)	2 (0%)	51	81
All	All	4472/6092 (73%)	4242 (95%)	226 (5%)	4 (0%)	54	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1623	THR
1	B	1623	THR
1	A	1577	THR
1	B	1577	THR

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	1904/2547 (75%)	1847 (97%)	57 (3%)	41	73
1	B	1904/2547 (75%)	1848 (97%)	56 (3%)	42	74
All	All	3808/5094 (75%)	3695 (97%)	113 (3%)	44	73

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	2387	GLN
1	B	619	SER
1	B	2362	GLU
1	B	1793	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2117	HIS
1	B	1757	HIS
1	B	386	HIS
1	B	946	HIS
1	A	2387	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 monosaccharides 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
2	NAP	A	3500	-	45,52,52	2.66	15 (33%)	56,80,80	1.58	8 (14%)
2	NAP	B	3500	-	45,52,52	2.66	15 (33%)	56,80,80	1.58	8 (14%)

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	NAP	A	3500	-	-	8/31/67/67	0/5/5/5
2	NAP	B	3500	-	-	8/31/67/67	0/5/5/5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3500	NAP	O4B-C1B	8.66	1.53	1.41
2	A	3500	NAP	O4B-C1B	8.66	1.53	1.41
2	A	3500	NAP	C7N-N7N	6.57	1.45	1.33
2	B	3500	NAP	C7N-N7N	6.57	1.45	1.33
2	B	3500	NAP	C2N-N1N	6.49	1.42	1.35

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3500	NAP	C6N-N1N-C2N	-6.22	116.30	121.97
2	A	3500	NAP	C6N-N1N-C2N	-6.19	116.33	121.97
2	B	3500	NAP	C3D-C2D-C1D	3.95	106.93	100.98
2	A	3500	NAP	C3D-C2D-C1D	3.93	106.89	100.98
2	B	3500	NAP	PN-O3-PA	-2.85	123.04	132.83

There are no chirality outliers.

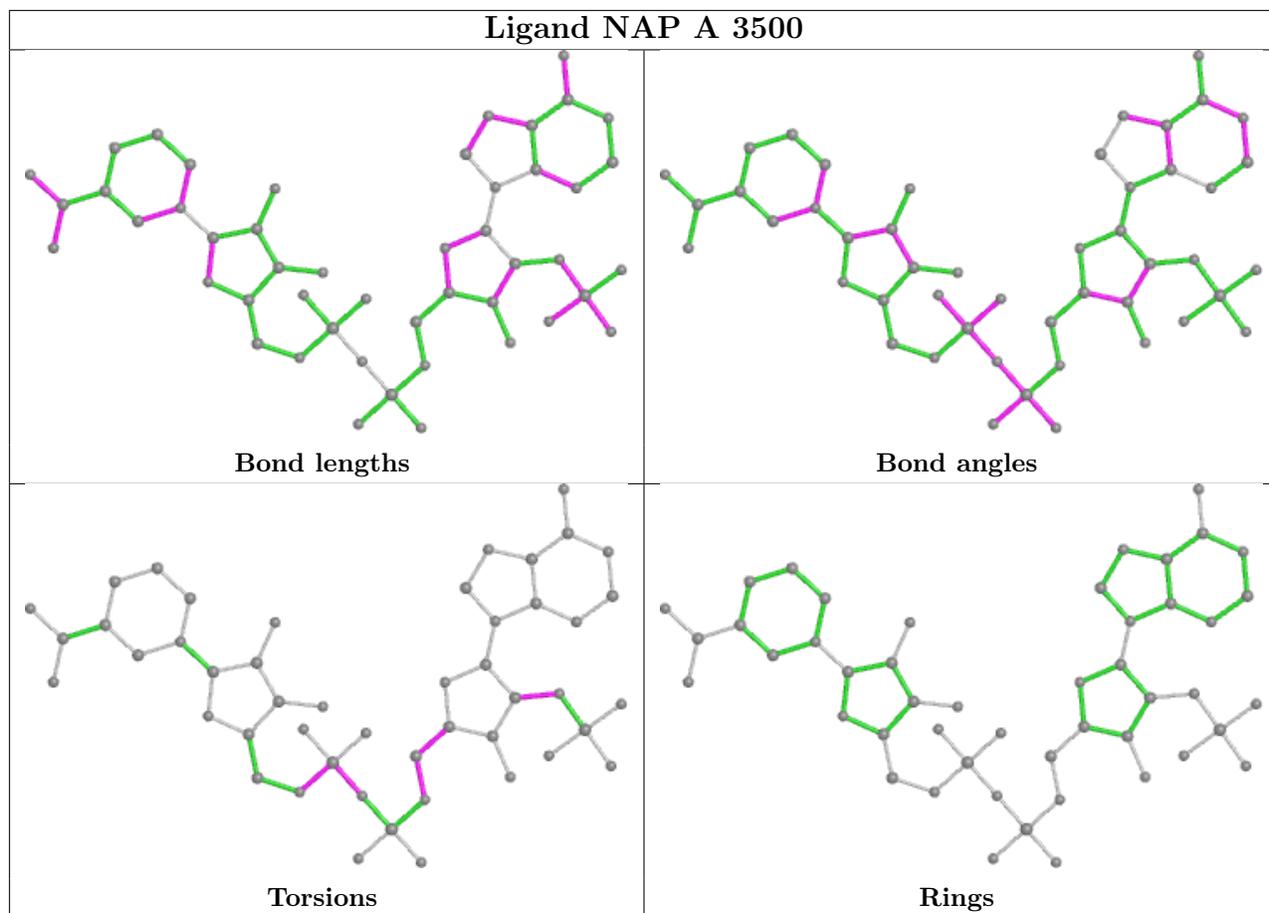
5 of 16 torsion outliers are listed below:

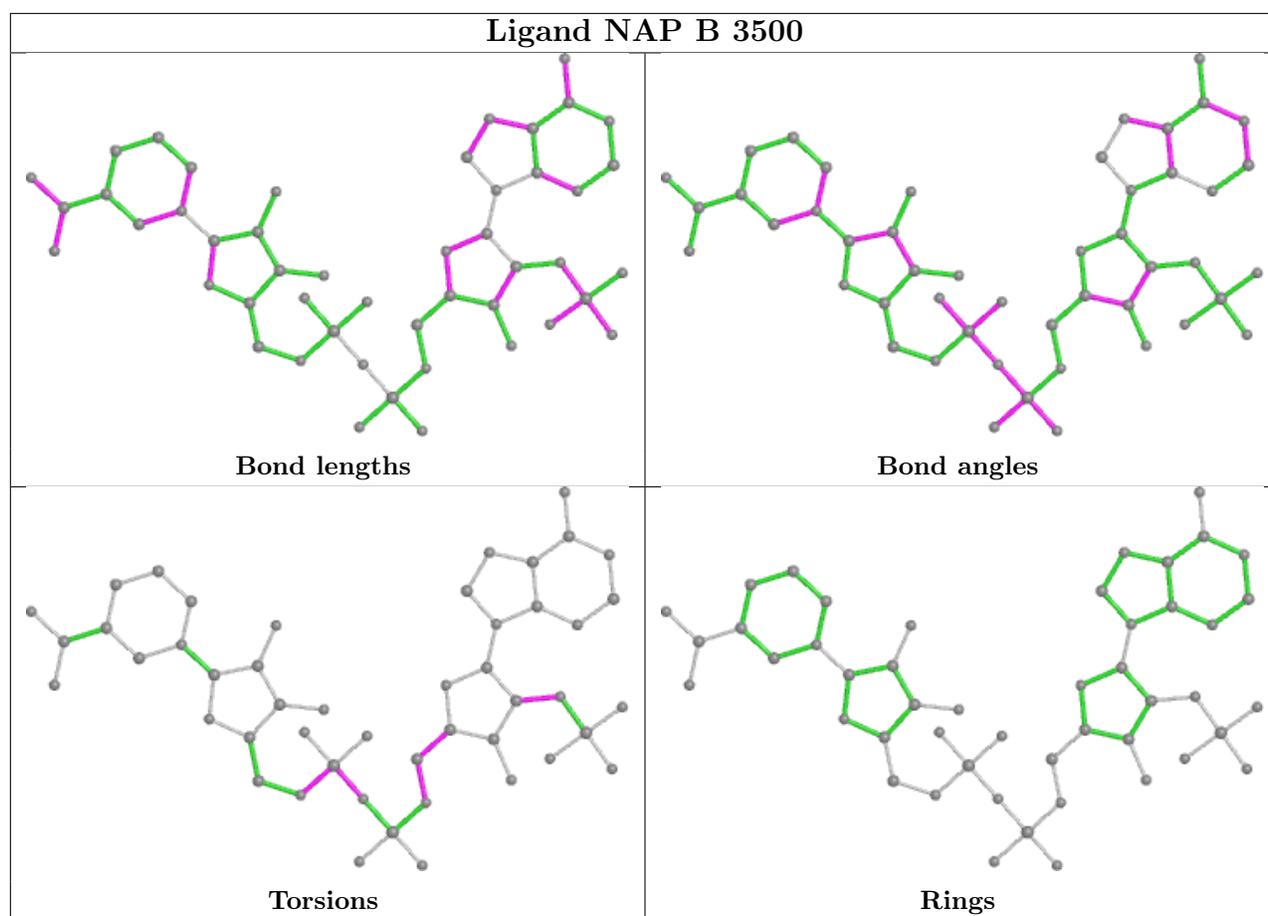
Mol	Chain	Res	Type	Atoms
2	A	3500	NAP	O4B-C4B-C5B-O5B
2	B	3500	NAP	O4B-C4B-C5B-O5B
2	A	3500	NAP	C1B-C2B-O2B-P2B
2	B	3500	NAP	C1B-C2B-O2B-P2B
2	A	3500	NAP	C3B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

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.

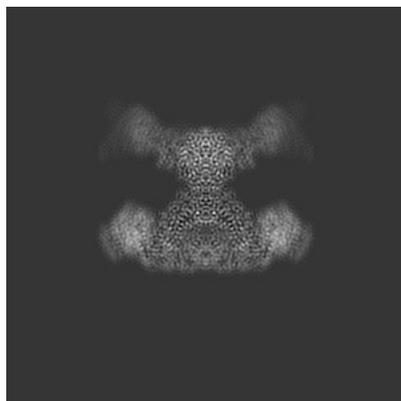
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30434. These allow visual inspection of the internal detail of the map and identification of artifacts.

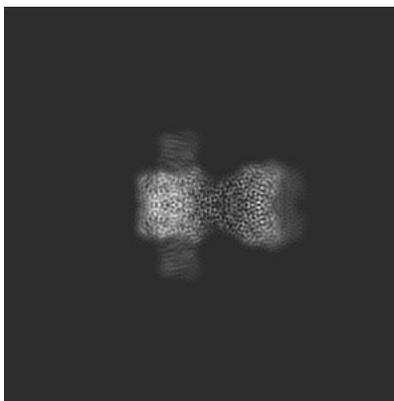
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

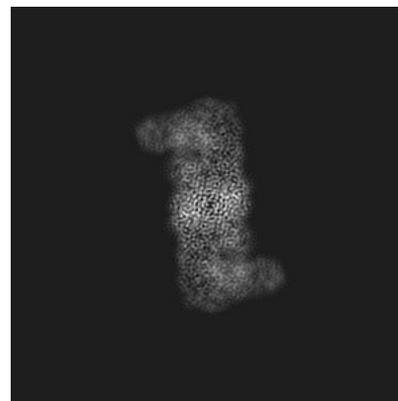
6.1.1 Primary map



X

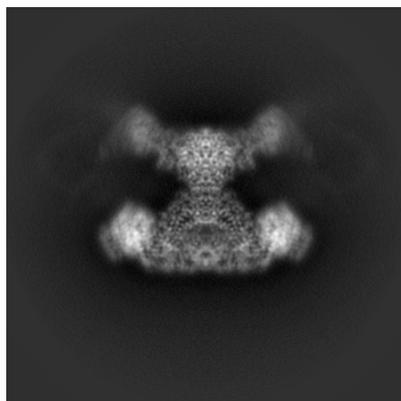


Y

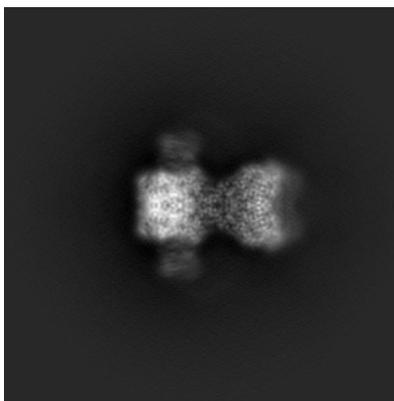


Z

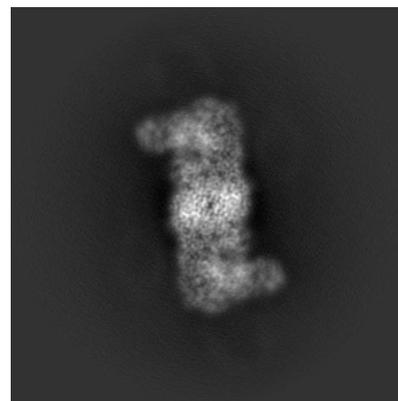
6.1.2 Raw map



X



Y

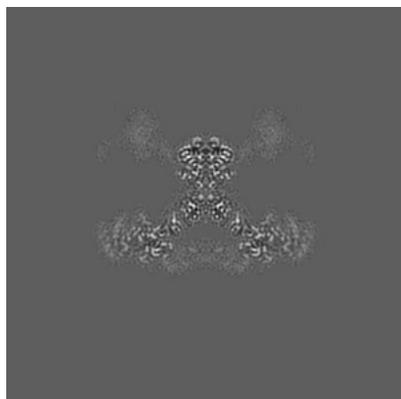


Z

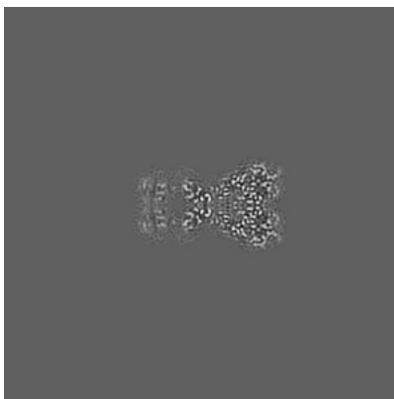
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

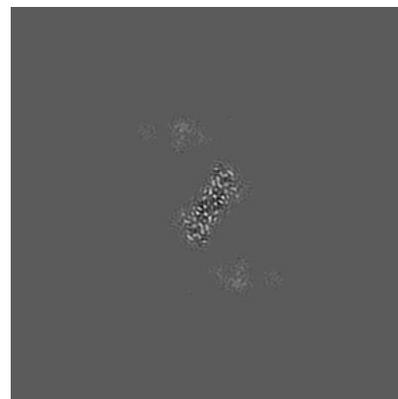
6.2.1 Primary map



X Index: 175

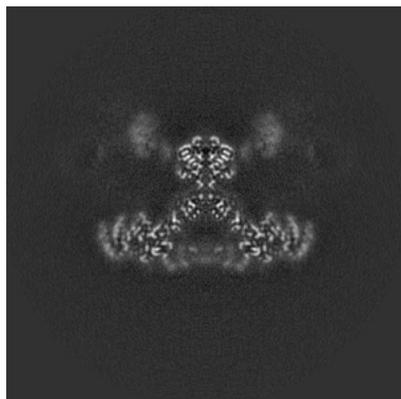


Y Index: 175

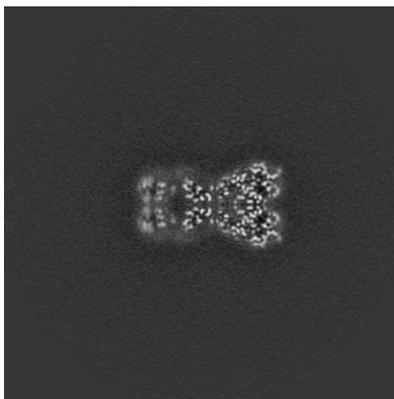


Z Index: 175

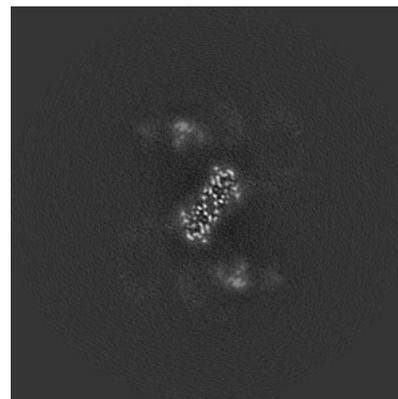
6.2.2 Raw map



X Index: 175



Y Index: 175

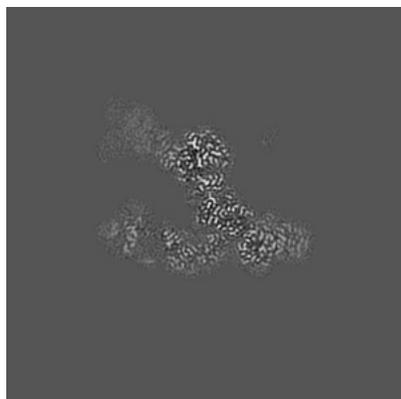


Z Index: 175

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: 185

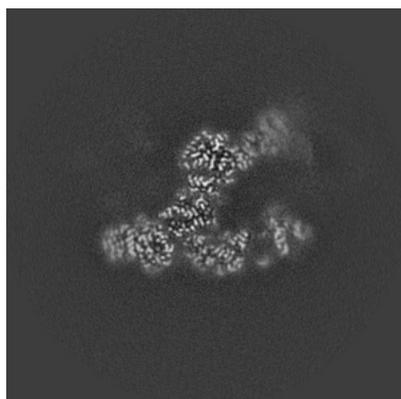


Y Index: 169

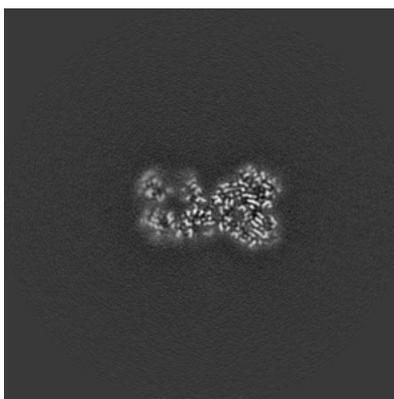


Z Index: 224

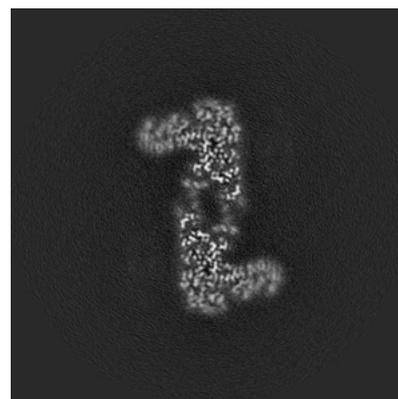
6.3.2 Raw map



X Index: 165



Y Index: 169

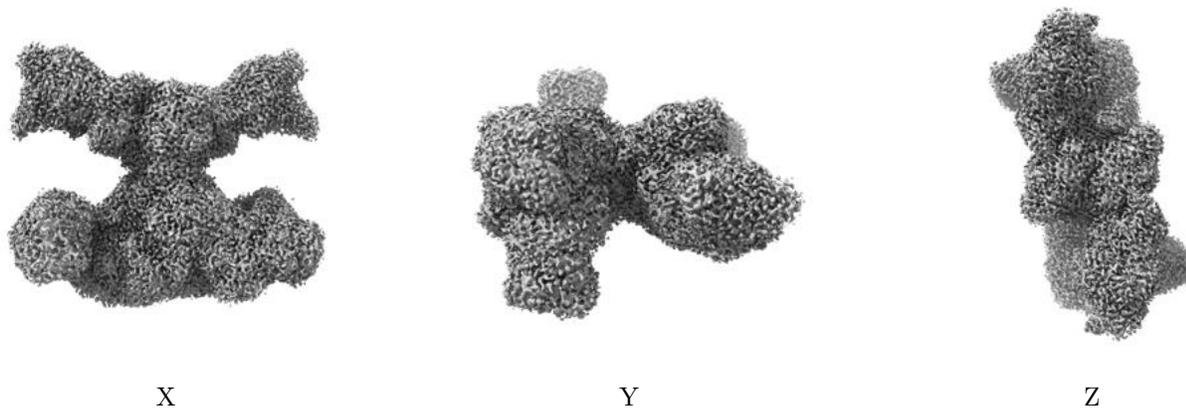


Z Index: 150

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

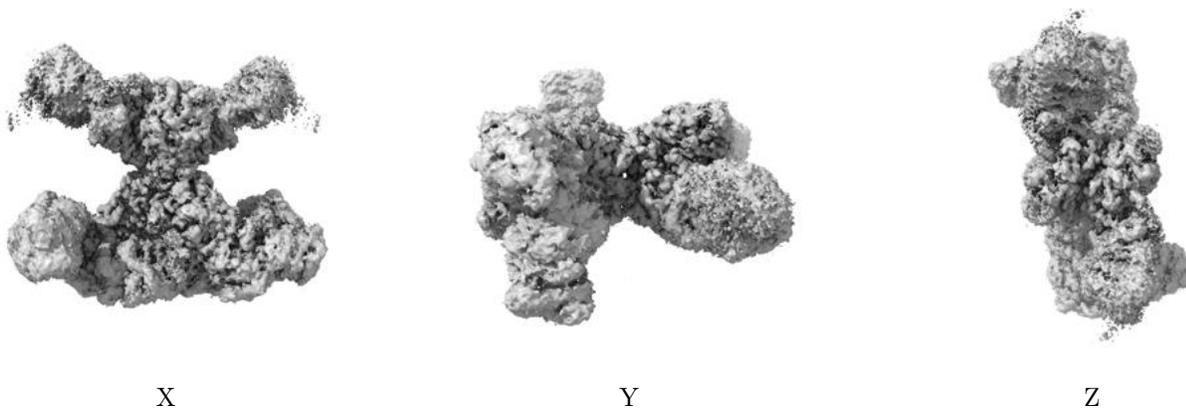
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

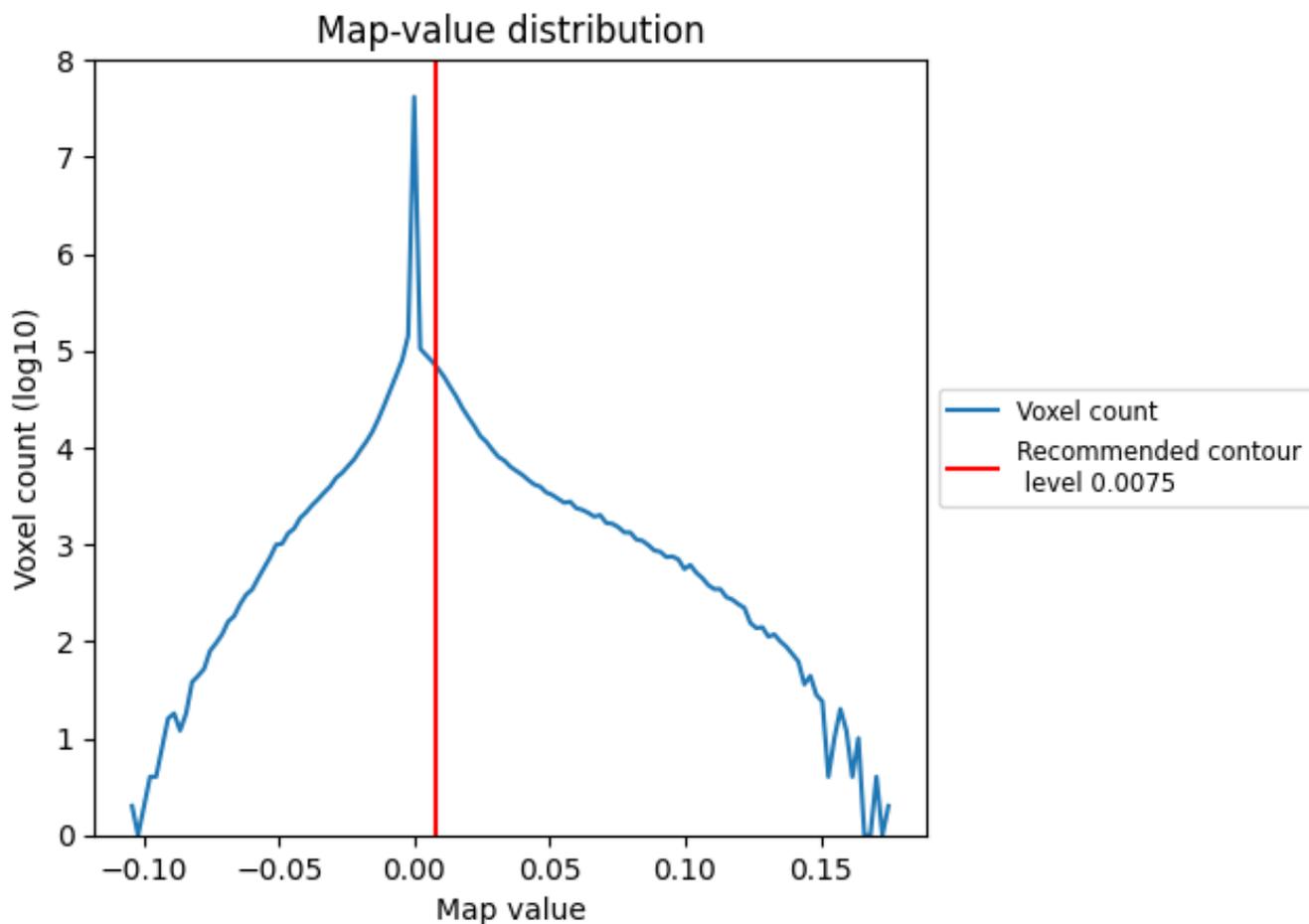
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

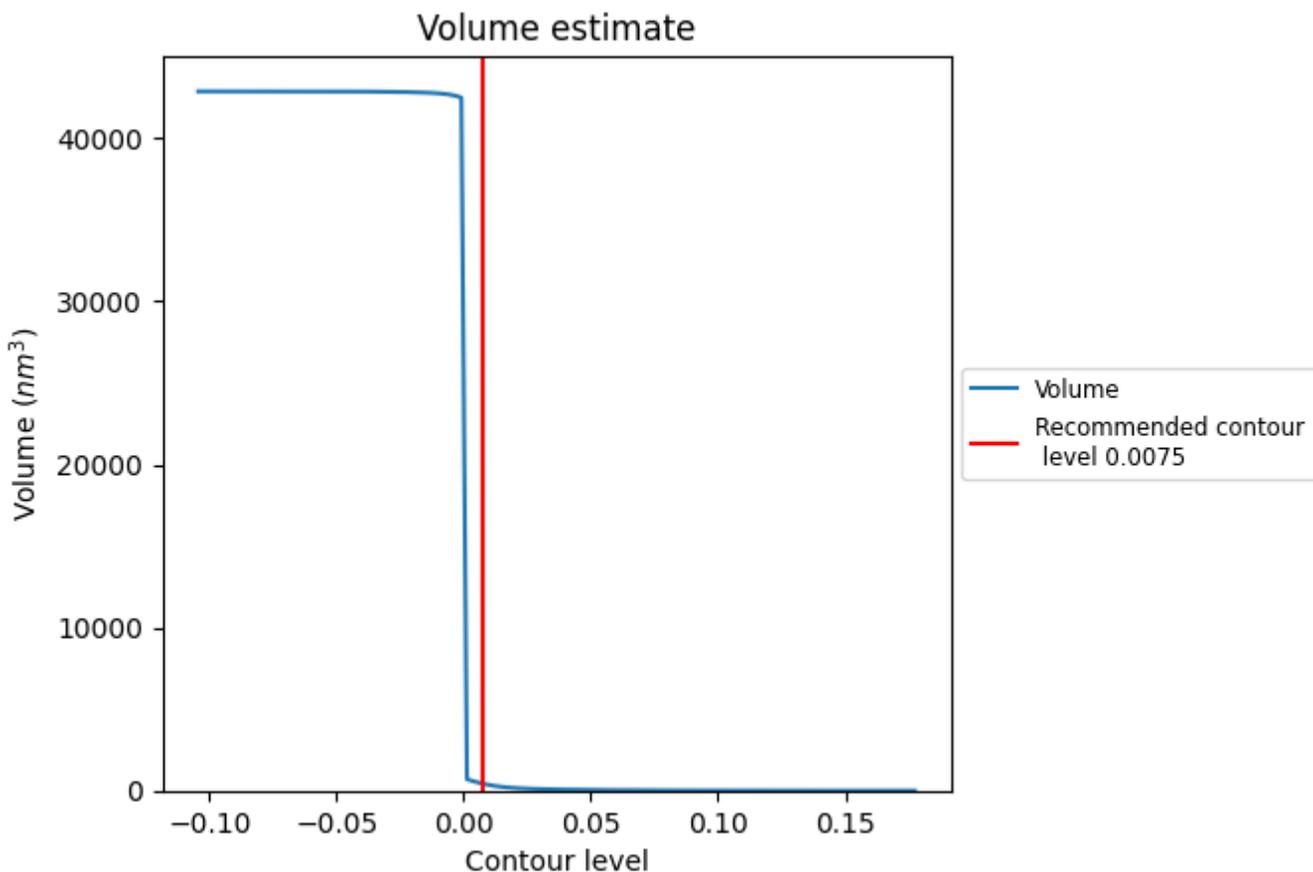
This section contains the results of statistical analysis of the map.

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.

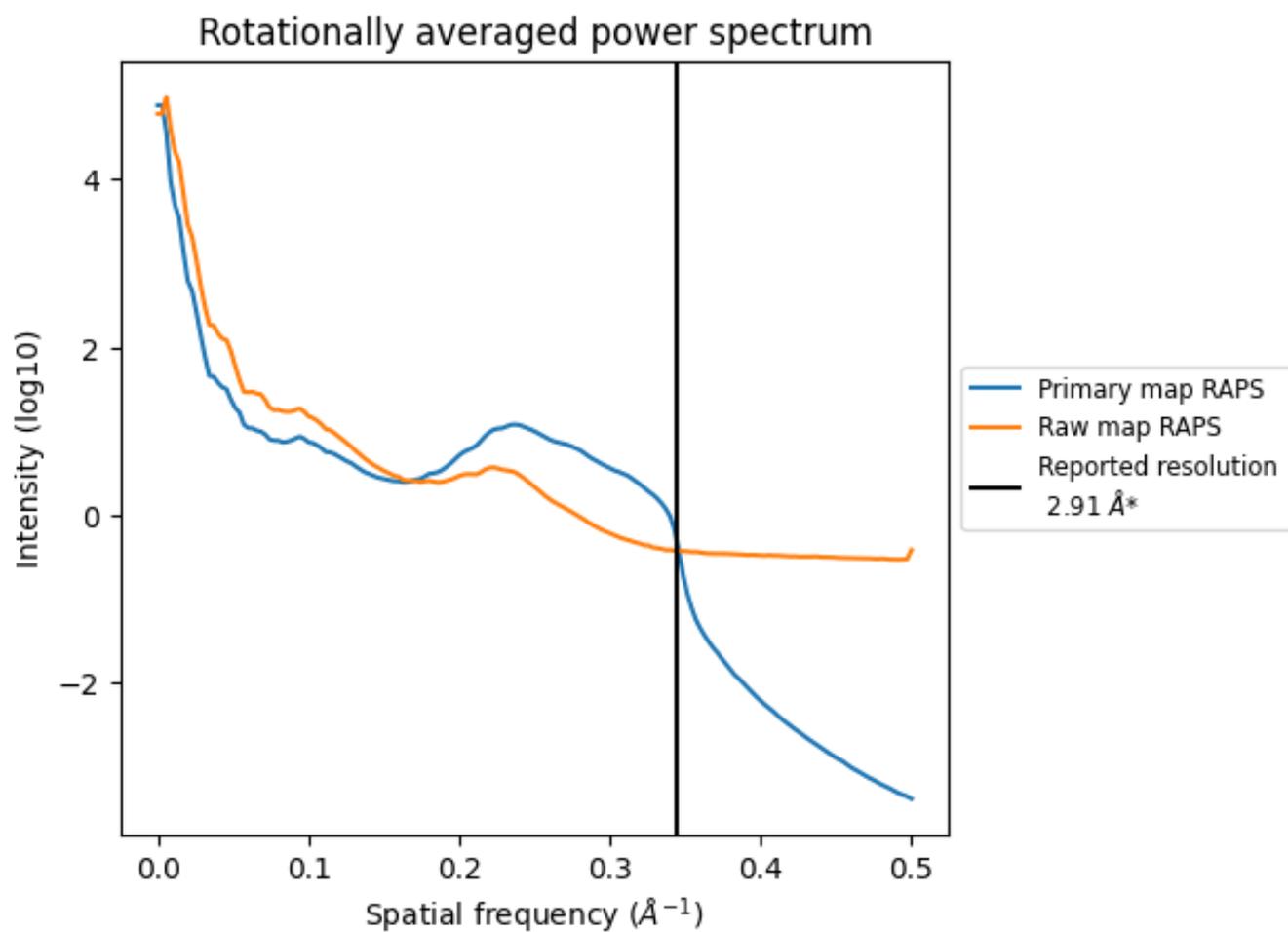
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 428 nm³; this corresponds to an approximate mass of 387 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

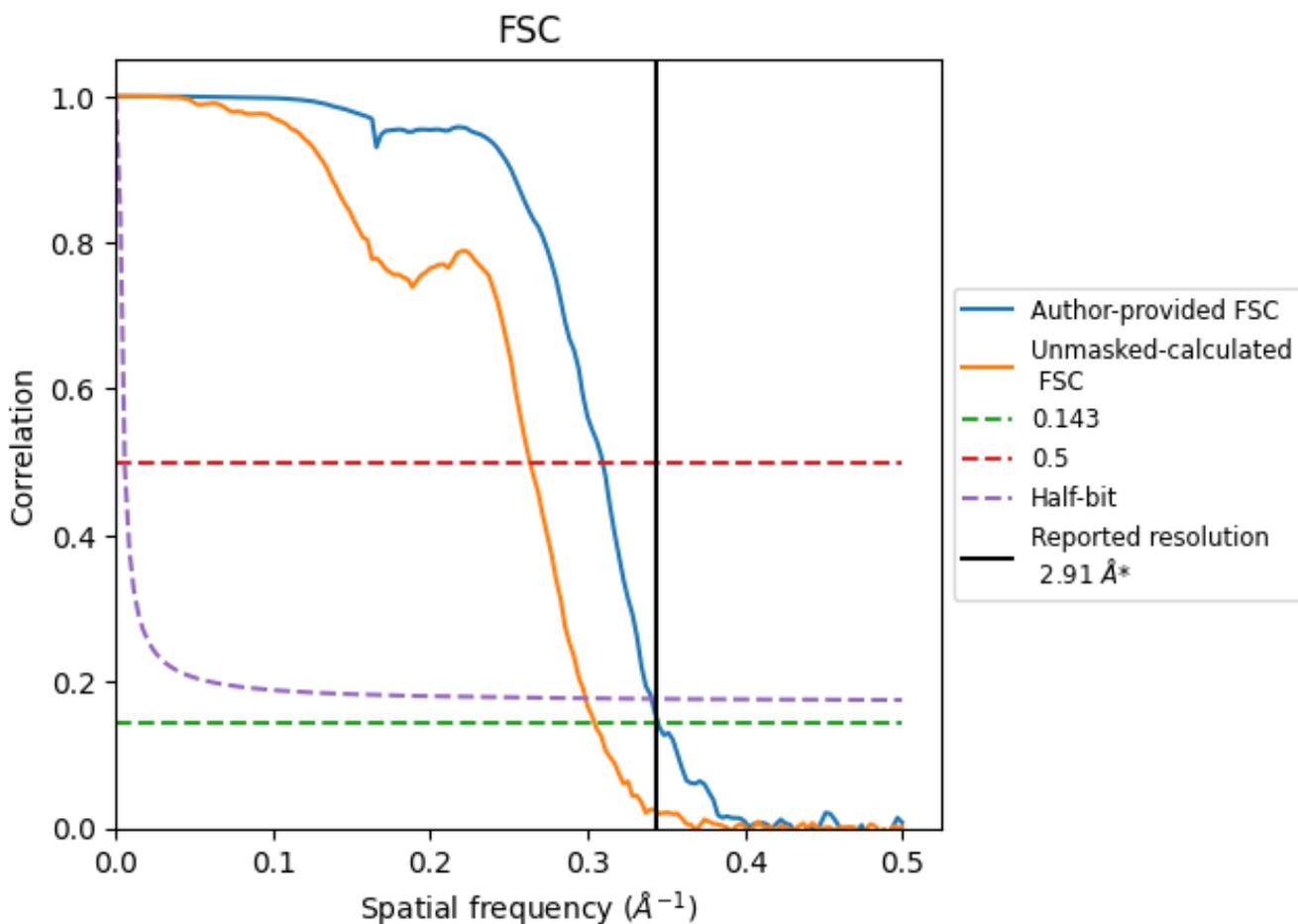


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

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 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

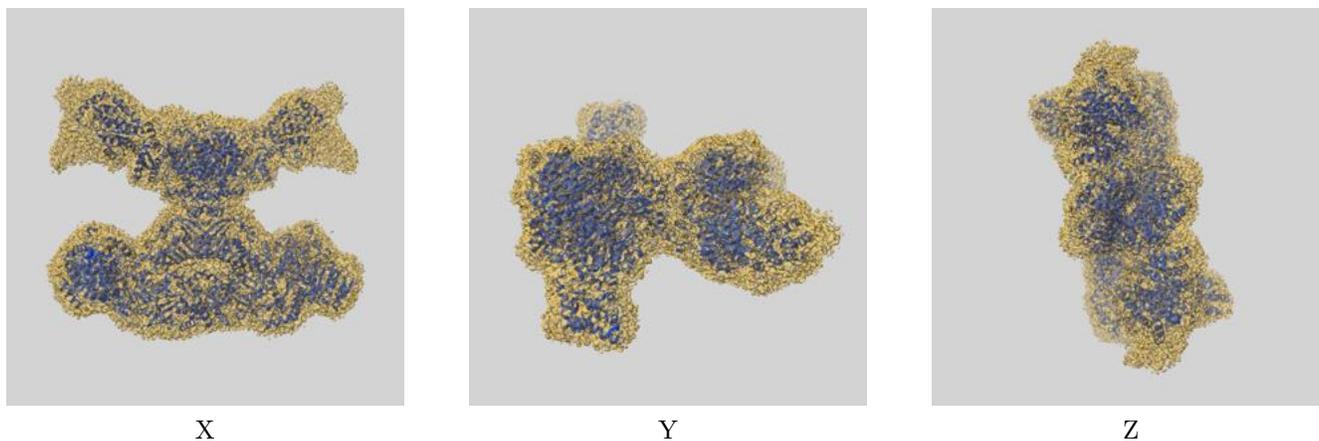
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.90	3.23	2.94
Unmasked-calculated*	3.28	3.80	3.35

*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 3.28 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

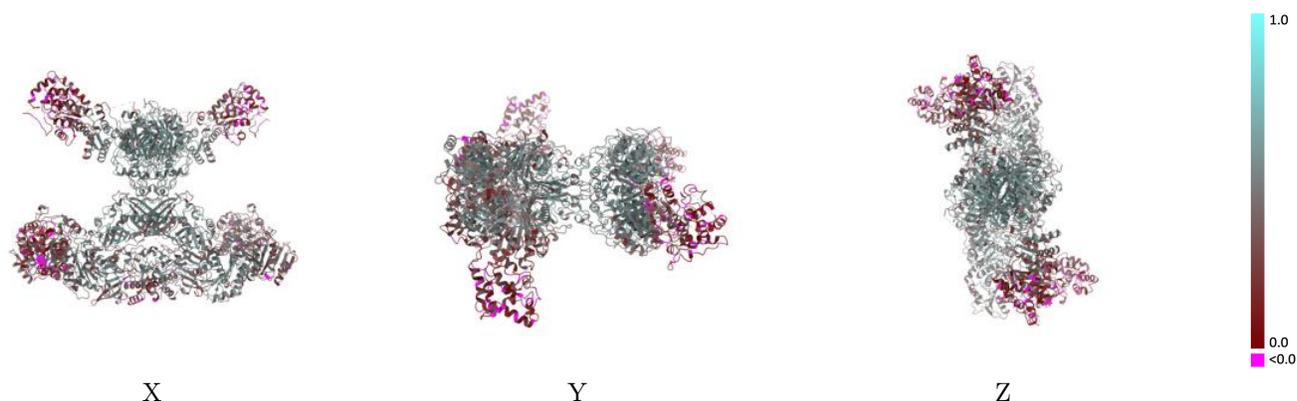
This section contains information regarding the fit between EMDB map EMD-30434 and PDB model 7CPX. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



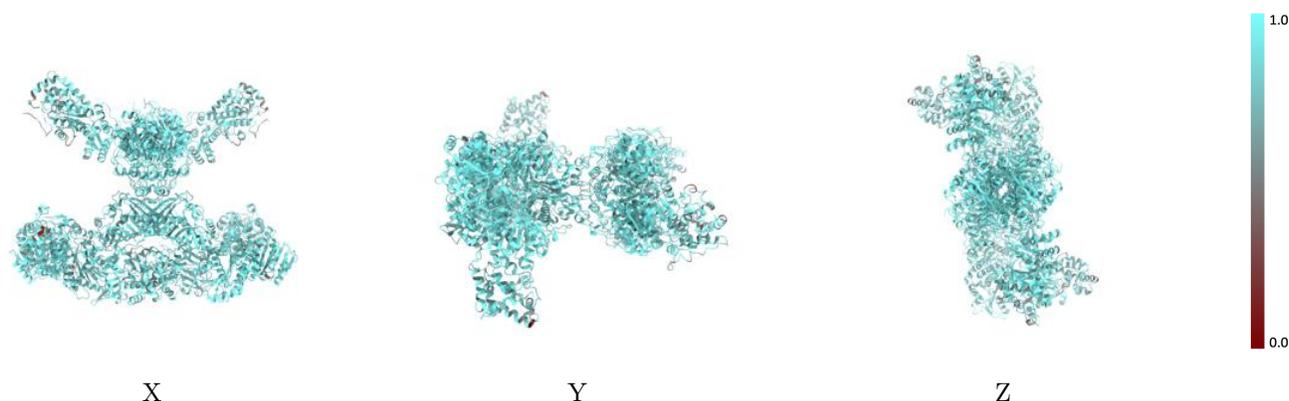
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



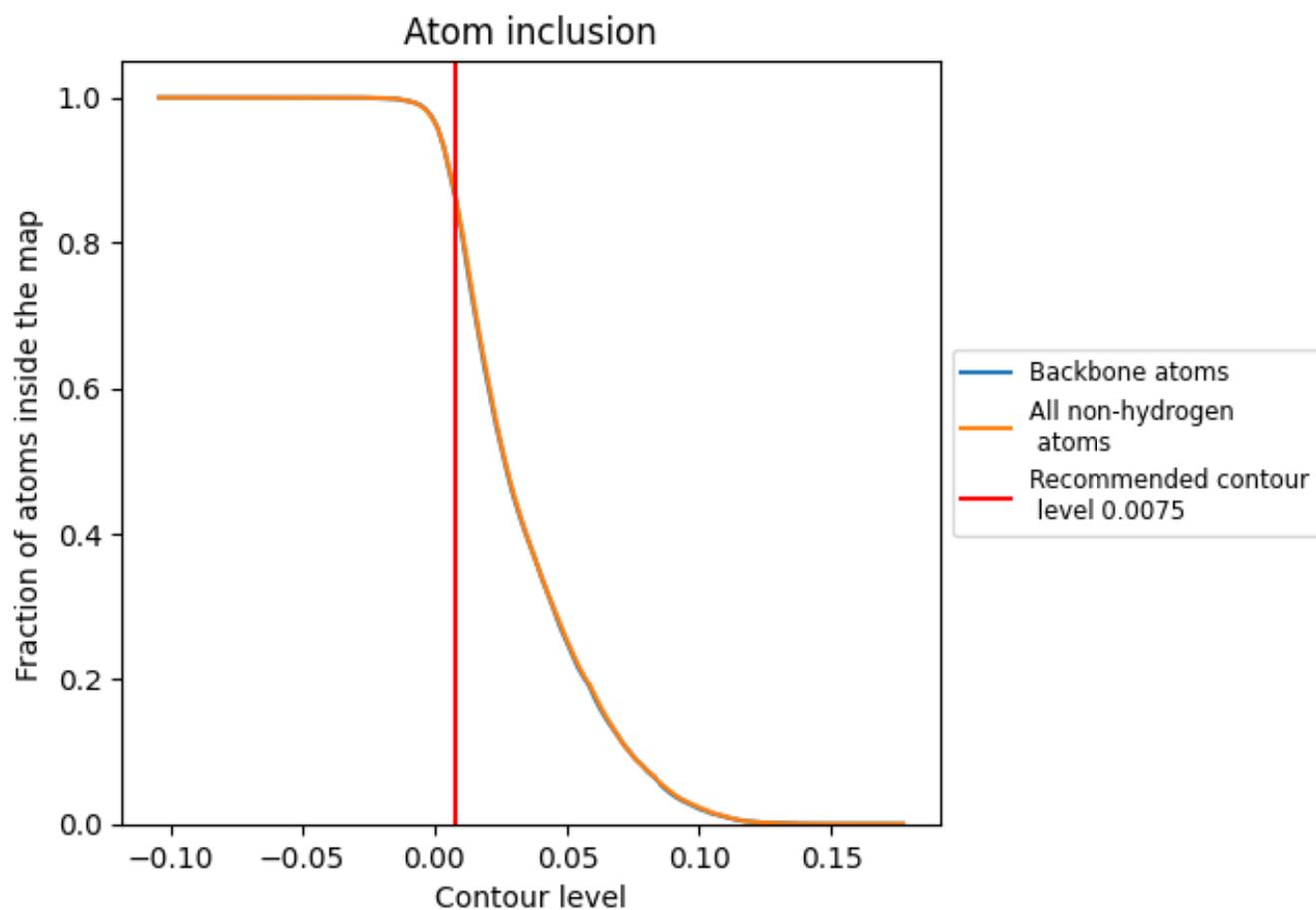
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8729	 0.4060
A	 0.8767	 0.4060
B	 0.8769	 0.4070

