



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 07:48 AM UTC

PDB ID : 8EYI / pdb_00008eyi
EMDB ID : EMD-28690
Title : Atomic model of the core modifying region of human fatty acid synthase
Authors : Hasan, S.M.N.; Keszei, A.; Mazhab-Jafari, M.T.
Deposited on : 2022-10-27
Resolution : 2.70 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

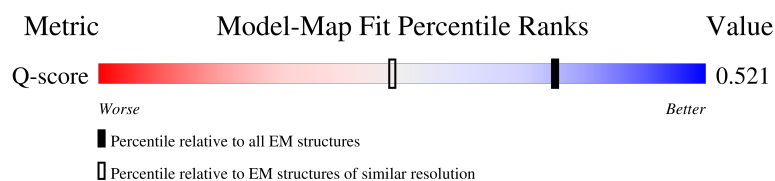
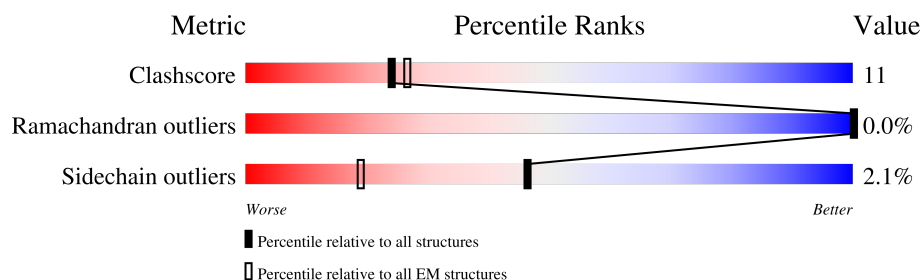
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

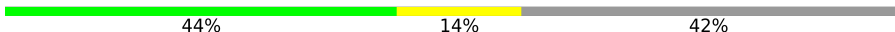
The reported resolution of this entry is 2.70 Å.

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	10327 (2.20 - 3.20)

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	E	1670	 44% 14% 42%
1	F	1670	 55% 17% 27%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16252 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.

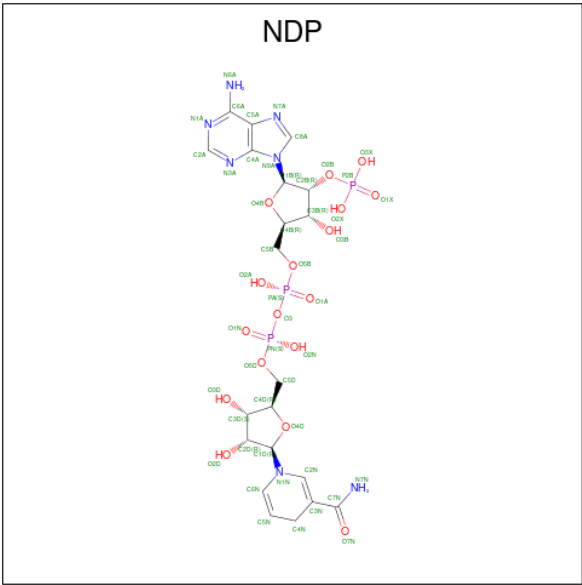
- Molecule 1 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	961	Total	C	N	O	S	0	0
			7150	4554	1263	1307	26		
1	F	1211	Total	C	N	O	S	0	0
			8910	5669	1574	1630	37		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	854	GLY	-	cloning artifact	UNP P49327
E	2512	LEU	-	cloning artifact	UNP P49327
E	2513	GLU	-	cloning artifact	UNP P49327
E	2514	SER	-	cloning artifact	UNP P49327
E	2515	ARG	-	cloning artifact	UNP P49327
E	2516	GLY	-	cloning artifact	UNP P49327
E	2517	PRO	-	cloning artifact	UNP P49327
E	2518	HIS	-	expression tag	UNP P49327
E	2519	HIS	-	expression tag	UNP P49327
E	2520	HIS	-	expression tag	UNP P49327
E	2521	HIS	-	expression tag	UNP P49327
E	2522	HIS	-	expression tag	UNP P49327
E	2523	HIS	-	expression tag	UNP P49327
F	854	GLY	-	cloning artifact	UNP P49327
F	2512	LEU	-	cloning artifact	UNP P49327
F	2513	GLU	-	cloning artifact	UNP P49327
F	2514	SER	-	cloning artifact	UNP P49327
F	2515	ARG	-	cloning artifact	UNP P49327
F	2516	GLY	-	cloning artifact	UNP P49327
F	2517	PRO	-	cloning artifact	UNP P49327
F	2518	HIS	-	expression tag	UNP P49327
F	2519	HIS	-	expression tag	UNP P49327
F	2520	HIS	-	expression tag	UNP P49327
F	2521	HIS	-	expression tag	UNP P49327
F	2522	HIS	-	expression tag	UNP P49327
F	2523	HIS	-	expression tag	UNP P49327

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	E	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	F	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	F	1	Total	C	N	O	P	0
			48	21	7	17	3	



GLU	VAL	VAL	ALA	ARG	PRO	VAL	R2043	TI905	SER	
PRO	MET	LEU	GLN	LEU	THR	ASN	R2043	R1905		
ARG	PRO	GLU	GLN	LEU	PRO	ASN	R1907	D1806		E1669
VAL	ARG	ALA	PRO	ILE	LYS	ASP	A2057	W1807		T1670
SER	LEU	LEU	SER	PRO	GLU	SER				
VAL	ALA	LEU	ALA	THR	ASP	SER	W2080	Q1910	Y1810	I1673
ARG	THR	PRO	THR	TYR	GLY	LEU		K1911		H1674
GLU	THR	LEU	GLY	GLY	LEU	ALA	I2063	L1912		S1675
GLY	GLY	LYS	ASN	LEU	ALA	ASP				
GLY	GLY	GLY	HIS	GLN	GLN	GLY	V2066	T1915	Y1823	G1679
GLU	ALA	LEU	SER	CYS	GLN	GLY	G2067	S1916	V1836	V1695
SER	TYR	GLU	LEU	THR	GLN	LEU	I2068	R1917		
ARG	GLY	GLU	PHE	ARG	THR	ASP	L2069	Y1924		K1704
GLY	GLU	ARG	LEU	ALA	GLN	SER	L2070	Q1925	F1831	
PRO	ASP	VAL	PHE	ALA	LEU	LEU	E2071	A1926		Q1709
HIS	HIS	LEU	ASP	PRO	ASN	MET		K1927	V1836	
GLY	GLY	ALA	GLY	LEU	LEU	SER			E1837	L1715
HIS	ALA	ALA	SER	ASP	ARG	VAL		R1933	D1836	
HIS	ASP	VAL	PRO	ILE	SER	GLU	L2084		A1839	F1720
HIS	TYR	ASP	THR	ILE	LEU	VAL		V1937		
HIS	ASN	LEU	TYR	HIS	LEU	ARG	Q1938	Q1938	M1843	R1724
	VAL	ILE	VAL	SER	VAL	GLN	A2089	V1939	A1844	
SER	SER	ILE	LEU	LEU	ASN	THR			Q1845	E1729
GLN	GLN	LYS	ALA	ALA	PRO	LEU	E2093	G1954	G1846	
VAL	VAL	SER	TYR	ALA	GLU	GLU			K1947	V1741
CYS	CYS	HIS	THR	ALA	GLY	ARG	V2105	E1958	H1848	
GLY	GLY	GLN	GLN	TYR	PRO	GLU				V1744
LYS	LYS	LEU	TYR	ILE	THR	LEU	V2110	V1968	V1852	
VAL	VAL	ASP	ARG	ASP	LEU	ASN	L2111			S1747
SER	SER	ARG	ALA	CYS	MET	LEU	A2112	V1973	V1856	
VAL	VAL	GLN	LYS	ARG	ARG	VAL	GLU	V1974	E1751	E1751
HIS	HIS	GLU	LEU	GLN	ASN	LEU	LYS	L1975	E1860	K1752
VAL	VAL	LEU	THR	VAL	SER	VAL	ALA	R1976		
ILE	ILE	SER	PRO	GLN	VAL	ARG	ALA	D1977	K1866	S1756
GLU	GLY	PHE	GLY	PRO	GLU	GLU	TYR	G1978	GLY	
GLY	ALA	ALA	CYS	GLY	SER	VAL	ALA		ALA	C1759
ASP	HIS	ARG	ALA	PRO	GLU	GLN	ASP	V1991	LYS	L1760
ARG	ARG	GLU	GLU	TYR	ARG	LEU	ASP	K1995	PRO	R1765
THR	THR	PHE	ALA	ARG	PRO	THR	ASP		K1871	F1766
LEU	LEU	TYR	THR	VAL	LEU	LEU	SER	T1999		L1767
GLU	GLU	THR	ALA	ALA	PHE	ARG	GLN		S1877	E1768
LYS	LYS	GLY	GLY	GLY	LEU	LYS	ASP	E2012	K1876	I1769
GLY	GLY	LEU	ALA	TYR	VAL	LEU	LEU	L2013	T1879	
SER	SER	ARG	ILE	SER	HIS	GLN	VAL	F2016		L1774
GLY	GLY	ALA	PHE	TYR	PRO	GLU	GLU		A1882	
LEU	LEU	PHE	CYS	GLY	ILE	LEU	GLU	S2021	H1883	L1780
GLU	GLU	PHE	ALA	ALA	GLU	LEU	ALA	V2022	K1885	M1781
ILE	ILE	VAL	VAL	CYS	GLY	SER	VAL			M1782
ILE	ILE	TYR	GLN	VAL	SER	LYS	ALA	E2023	I1888	L1786
ILE	ILE	GLN	GLN	ALA	THR	ALA	HIS	C2024	I1889	
SER	SER	PHE	PHE	PHE	THR	ASP	ILE		A1890	
LYS	LYS	THR	THR	GLU	VAL	GLY	GLY	N2028		I1790
ILE	ILE	ALA	ASP	GLU	PHE	ALA	GLY	A2029	L1893	
HIS	HIS	LYS	MET	CYS	THR	ALA	ILE	G2030		G1793
SER	SER	TYR	GLU	VAL	HIS	SER	ARG	Q2031	L1898	V1794
SER	SER	HIS	GLU	SER	LEU	GLU	ASP	S2032		L1795
LEU	LEU	GLY	ASN	LEU	LEU	LEU	LEU		A1901	
ALA	ALA	ASN	ARG	GLN	SER	CYS	ALA	N2038		E1802
								S2039		SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	355649	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 ($e^-/\text{\AA}^2$)	50.76	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.083	Depositor
Minimum map value	-2.433	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.422	Depositor
Map size ($\text{\AA}$)	257.5, 257.5, 257.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.03, 1.03, 1.03	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: NDP

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	E	0.14	0/7315	0.29	0/9974
1	F	0.13	0/9106	0.31	1/12421 (0.0%)
All	All	0.13	0/16421	0.30	1/22395 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	977	PRO	CA-N-CD	-5.44	104.39	112.00

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	E	7150	0	6876	161	0
1	F	8910	0	8579	192	0
2	E	96	0	48	8	0
2	F	96	0	49	16	0
All	All	16252	0	15552	343	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 11.

The worst 5 of 343 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:F:1915:THR:HG22	2:F:3002:NDP:H2A	1.36	1.03
1:F:1576:ILE:HD13	1:F:1843:MET:HE2	1.61	0.83
1:F:1805:ALA:C	1:F:1807:TRP:H	1.87	0.83
1:E:2024:CYS:HG	1:E:2039:SER:HG	1.26	0.79
1:E:1991:VAL:HG11	1:E:2033:ASN:HB2	1.63	0.79

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	E	955/1670 (57%)	933 (98%)	22 (2%)	0	100	100
1	F	1199/1670 (72%)	1177 (98%)	21 (2%)	1 (0%)	48	73
All	All	2154/3340 (64%)	2110 (98%)	43 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1806	ASP

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	E	717/1392 (52%)	703 (98%)	14 (2%)	48	76
1	F	887/1392 (64%)	868 (98%)	19 (2%)	47	75
All	All	1604/2784 (58%)	1571 (98%)	33 (2%)	46	75

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1915	THR
1	F	1991	VAL
1	F	2032	SER
1	E	1980	LEU
1	E	1941	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1106	GLN
1	F	1331	ASN
1	F	2031	GLN
1	F	1935	GLN
1	F	1940	GLN

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 ⓘ

4 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	NDP	F	3002	-	51,52,52	3.66	23 (45%)	71,80,80	2.00	18 (25%)
2	NDP	F	3001	-	51,52,52	3.65	23 (45%)	71,80,80	1.93	12 (16%)
2	NDP	E	3002	-	51,52,52	3.65	21 (41%)	71,80,80	1.99	19 (26%)
2	NDP	E	3001	-	51,52,52	3.62	20 (39%)	71,80,80	1.87	17 (23%)

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	NDP	F	3002	-	-	14/34/77/77	0/5/5/5
2	NDP	F	3001	-	-	10/34/77/77	0/5/5/5
2	NDP	E	3002	-	-	8/34/77/77	0/5/5/5
2	NDP	E	3001	-	-	14/34/77/77	0/5/5/5

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3002	NDP	C2B-C1B	-11.00	1.26	1.53
2	E	3002	NDP	C2B-C1B	-10.98	1.26	1.53
2	F	3002	NDP	C2D-C3D	-10.53	1.24	1.53
2	E	3001	NDP	C2B-C1B	-10.51	1.27	1.53
2	E	3001	NDP	C2D-C3D	-10.42	1.25	1.53

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3001	NDP	C5A-C4A-N3A	-6.23	118.14	126.72
2	F	3002	NDP	C5A-C4A-N3A	-6.23	118.14	126.72
2	E	3001	NDP	C5A-C4A-N3A	-5.62	118.98	126.72
2	F	3001	NDP	N3A-C2A-N1A	-5.59	120.12	128.58
2	F	3002	NDP	O4B-C1B-C2B	-5.37	97.35	106.59

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

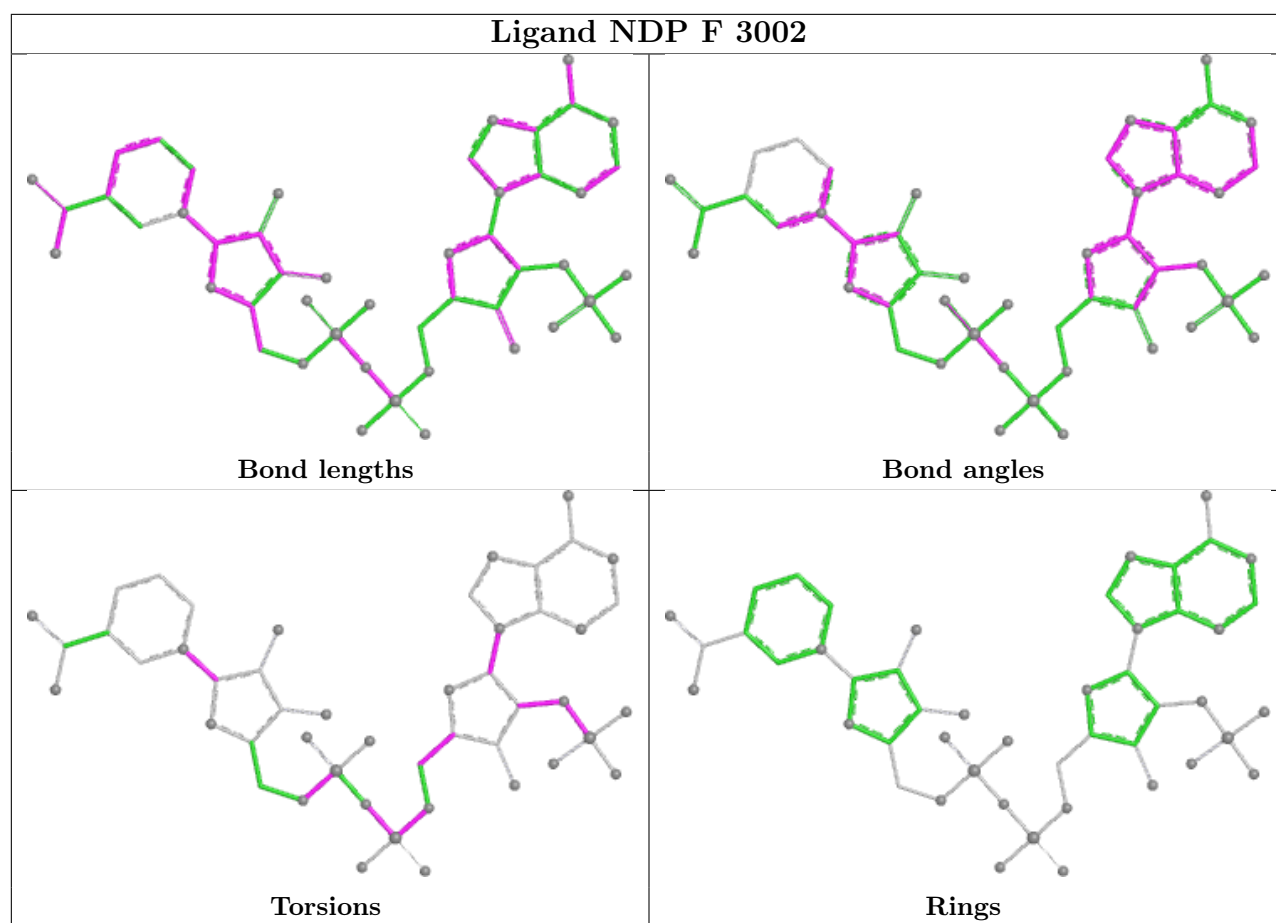
Mol	Chain	Res	Type	Atoms
2	E	3001	NDP	O4B-C4B-C5B-O5B
2	E	3002	NDP	C5B-O5B-PA-O1A
2	E	3002	NDP	C5B-O5B-PA-O3
2	E	3002	NDP	O4D-C1D-N1N-C6N
2	F	3001	NDP	C5B-O5B-PA-O3

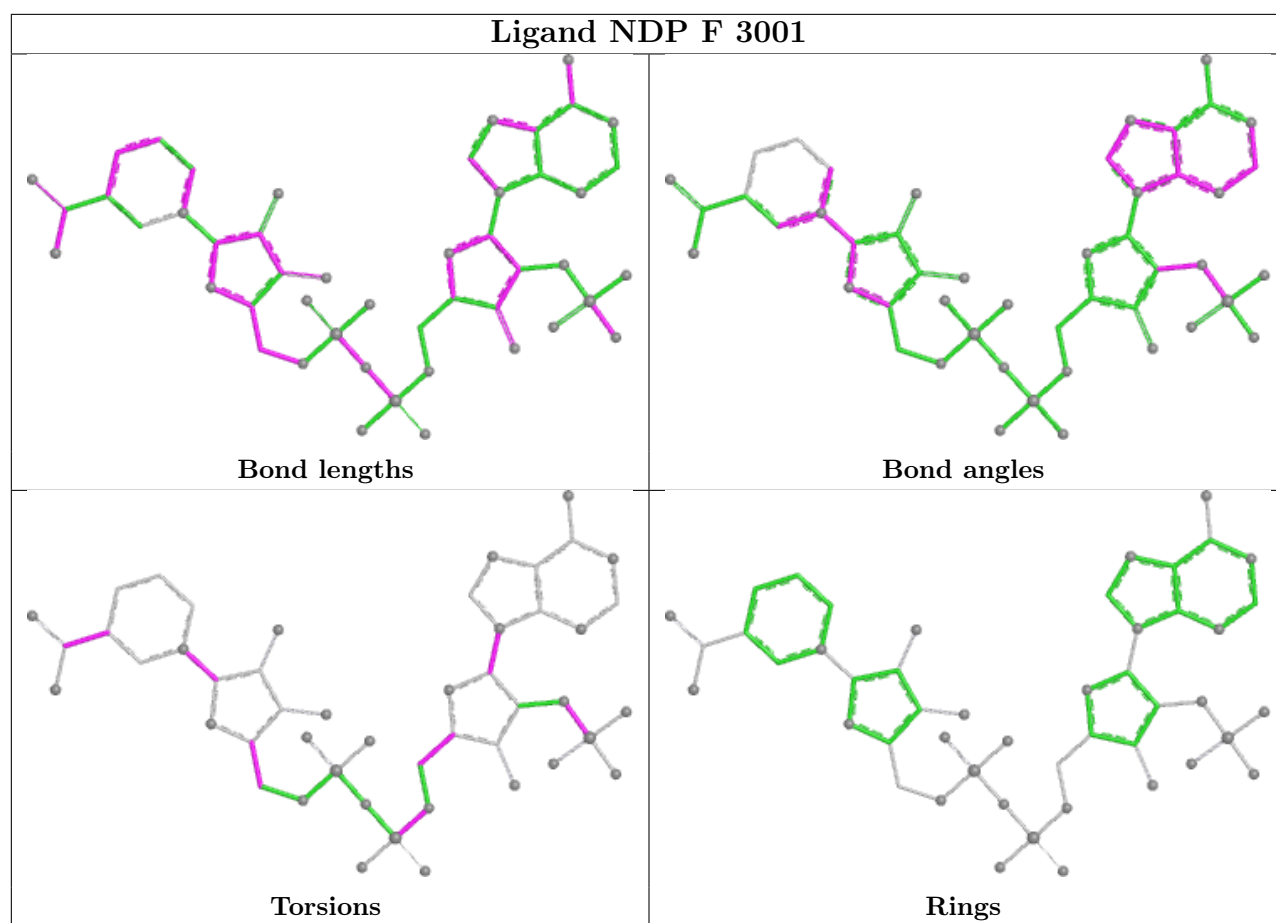
There are no ring outliers.

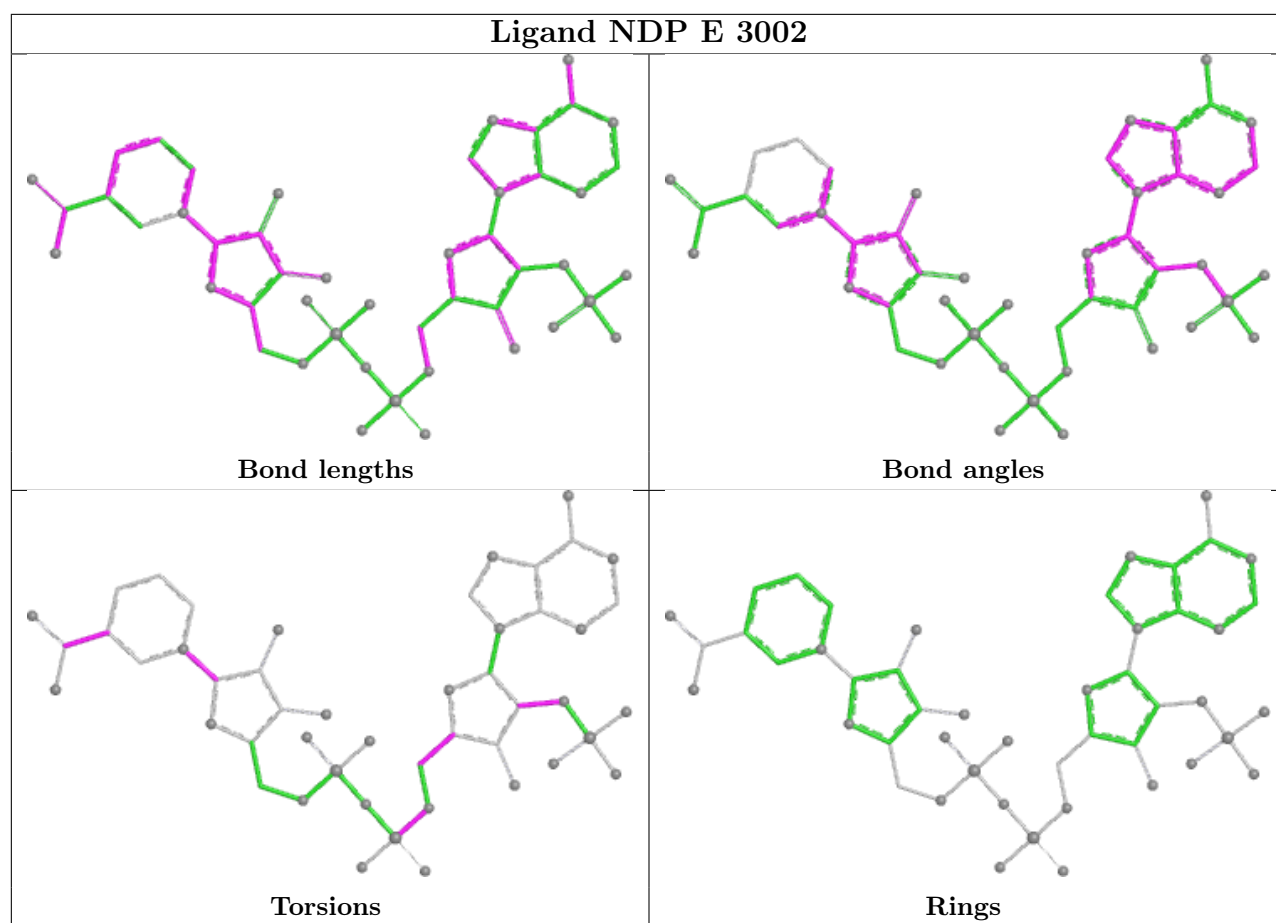
4 monomers are involved in 24 short contacts:

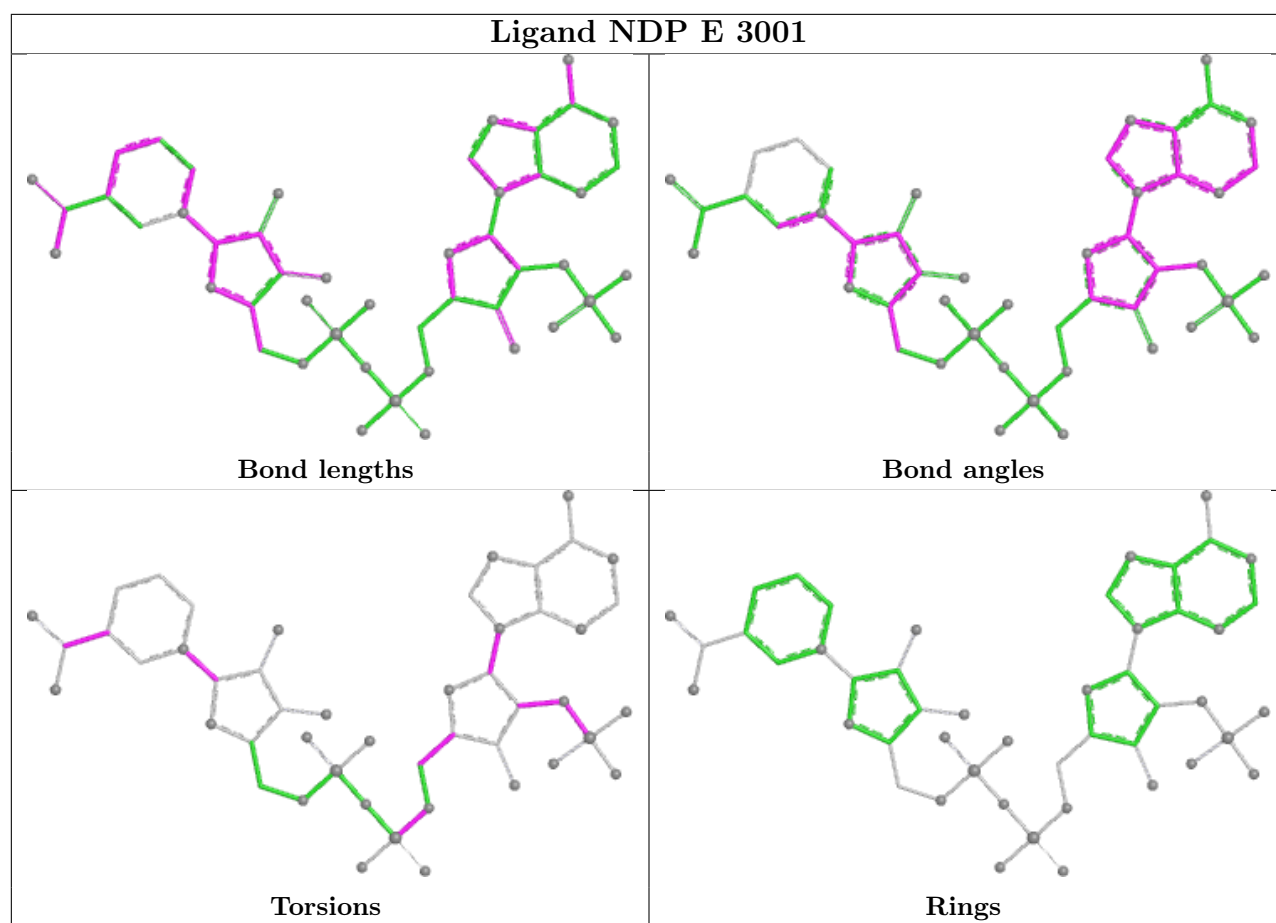
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3002	NDP	6	0
2	F	3001	NDP	10	0
2	E	3002	NDP	7	0
2	E	3001	NDP	1	0

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.

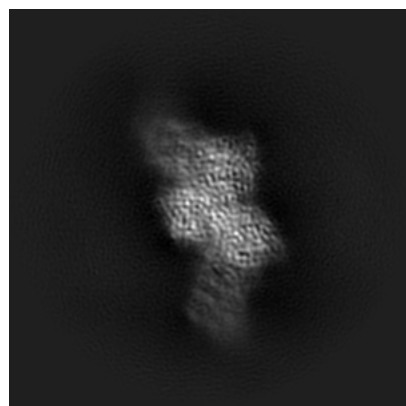
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28690. These allow visual inspection of the internal detail of the map and identification of artifacts.

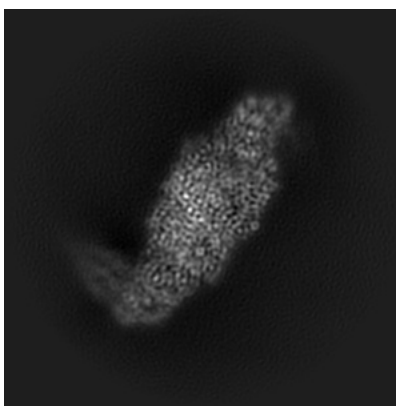
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

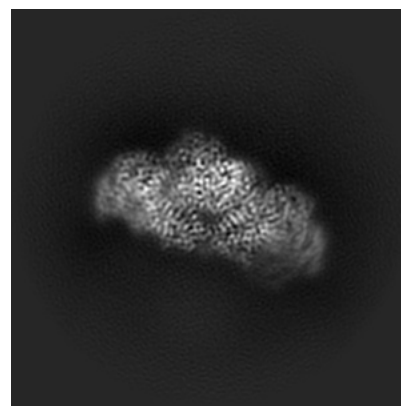
6.1.1 Primary map



X

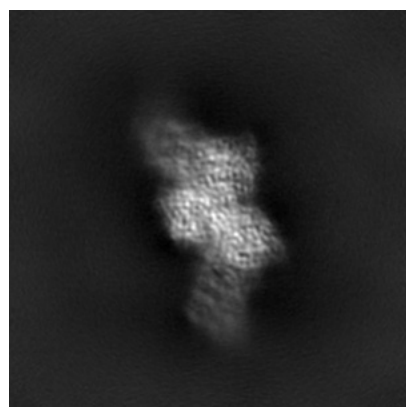


Y

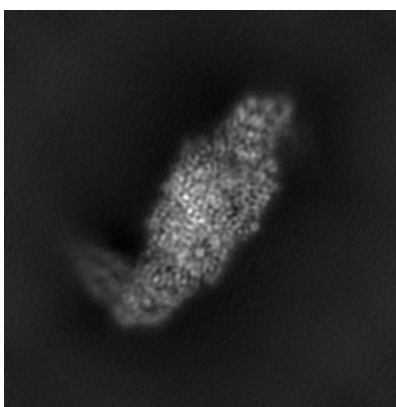


Z

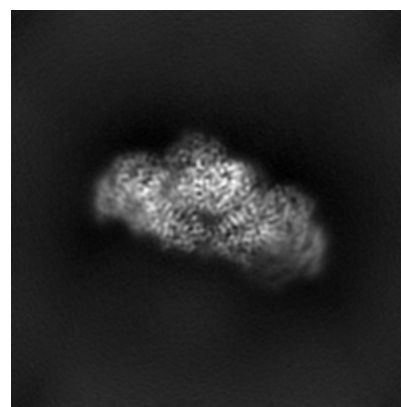
6.1.2 Raw map



X



Y

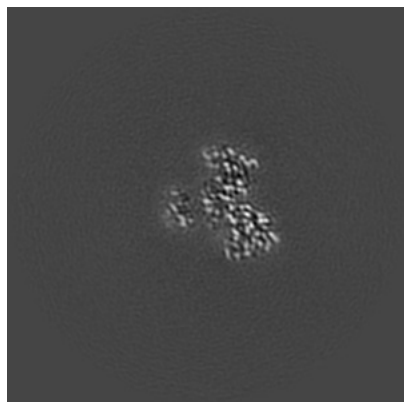


Z

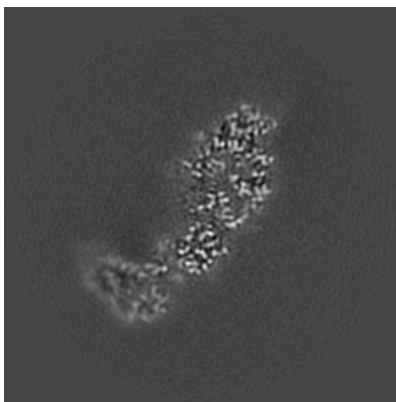
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

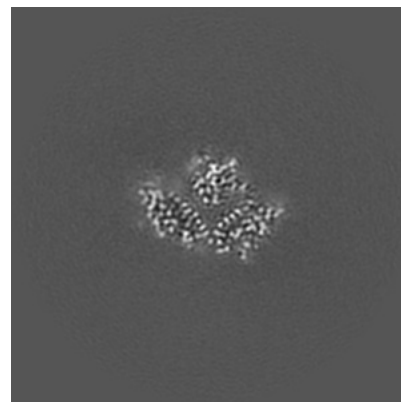
6.2.1 Primary map



X Index: 125

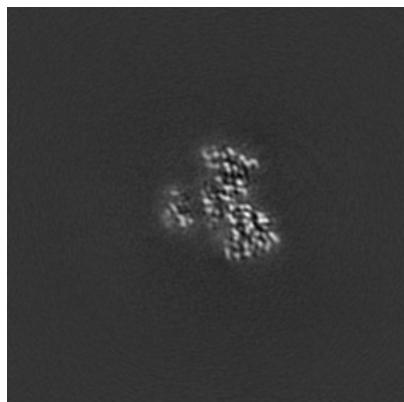


Y Index: 125

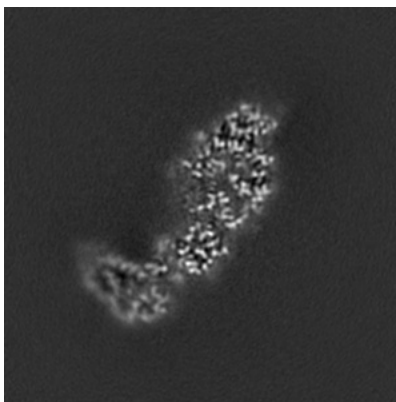


Z Index: 125

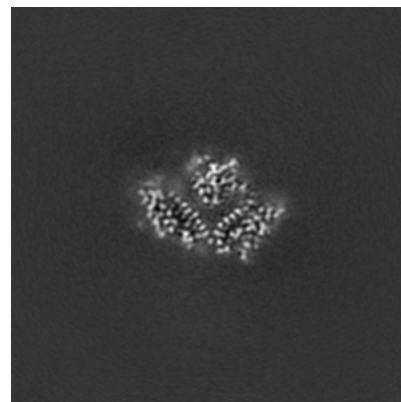
6.2.2 Raw map



X Index: 125



Y Index: 125

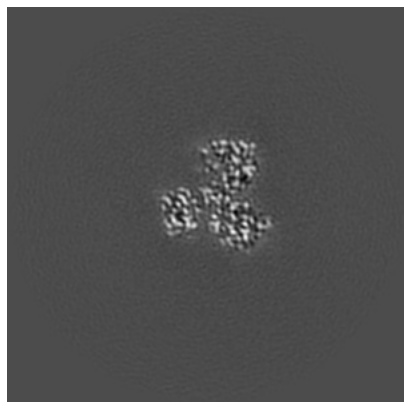


Z Index: 125

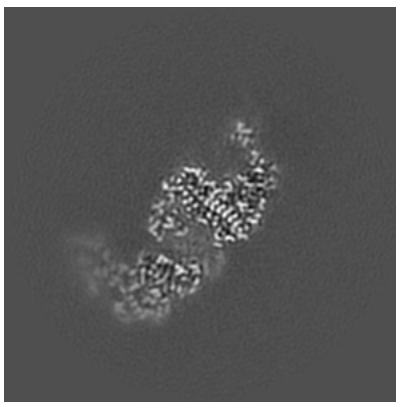
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

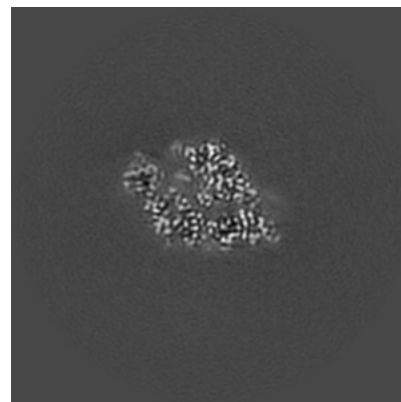
6.3.1 Primary map



X Index: 132

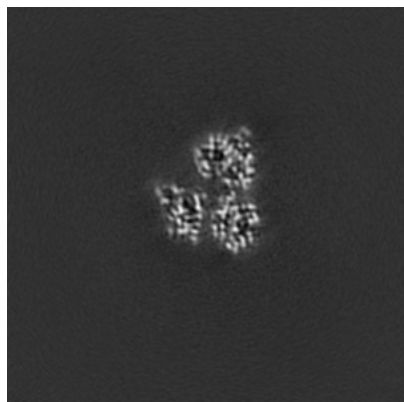


Y Index: 138

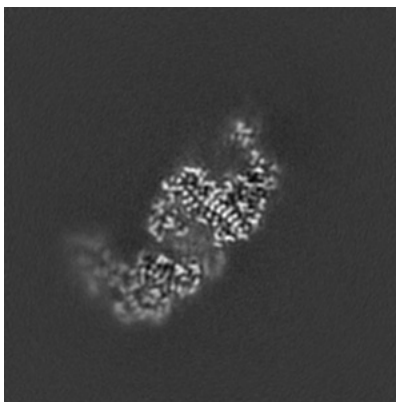


Z Index: 116

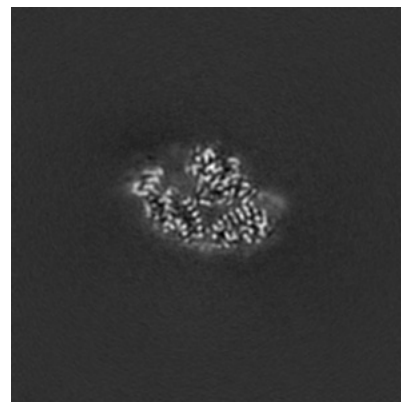
6.3.2 Raw map



X Index: 138



Y Index: 138

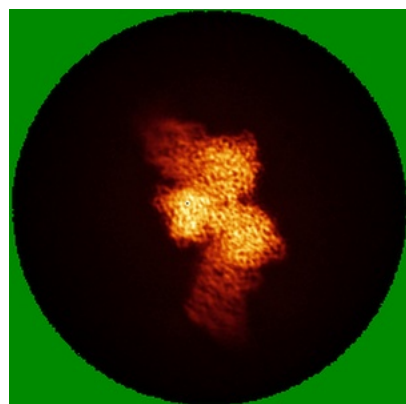


Z Index: 120

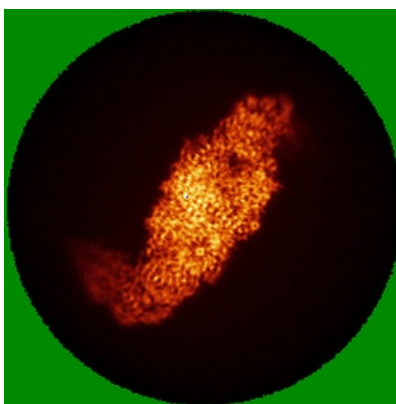
The images above show the largest variance slices of the map in three orthogonal directions.

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

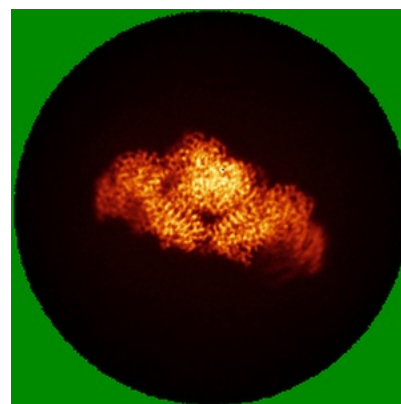
6.4.1 Primary map



X

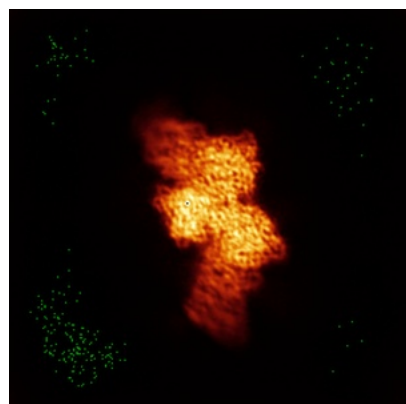


Y

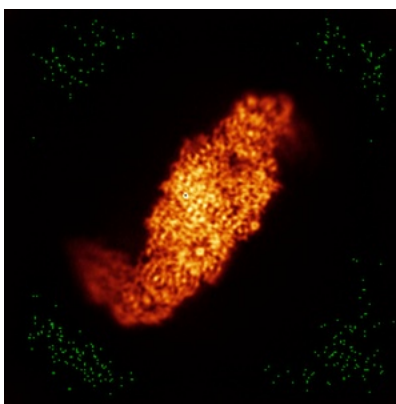


Z

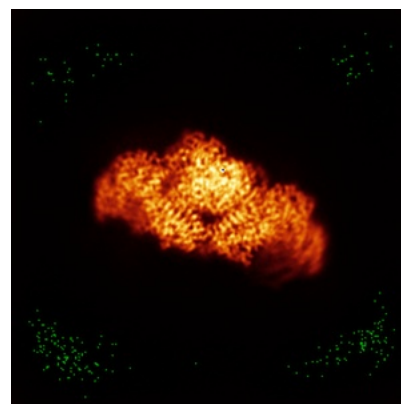
6.4.2 Raw map



X



Y

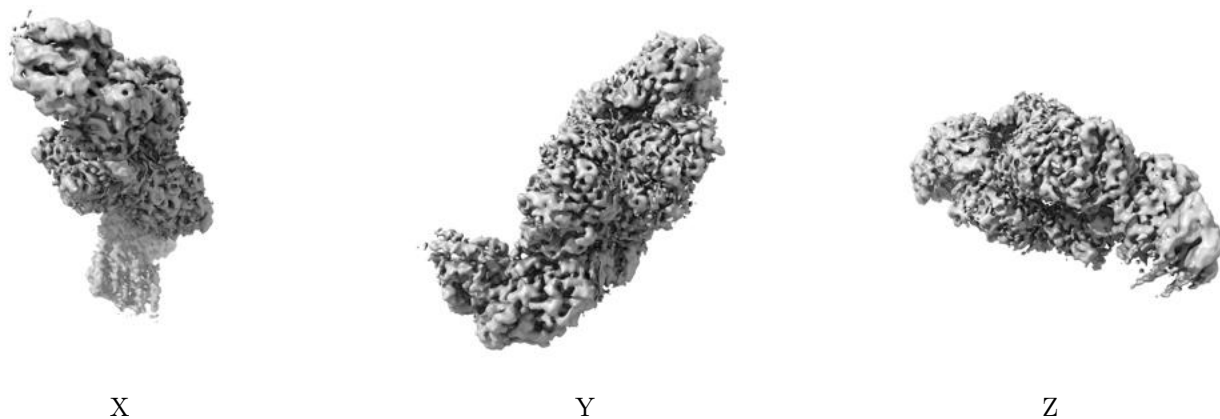


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.422. 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



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

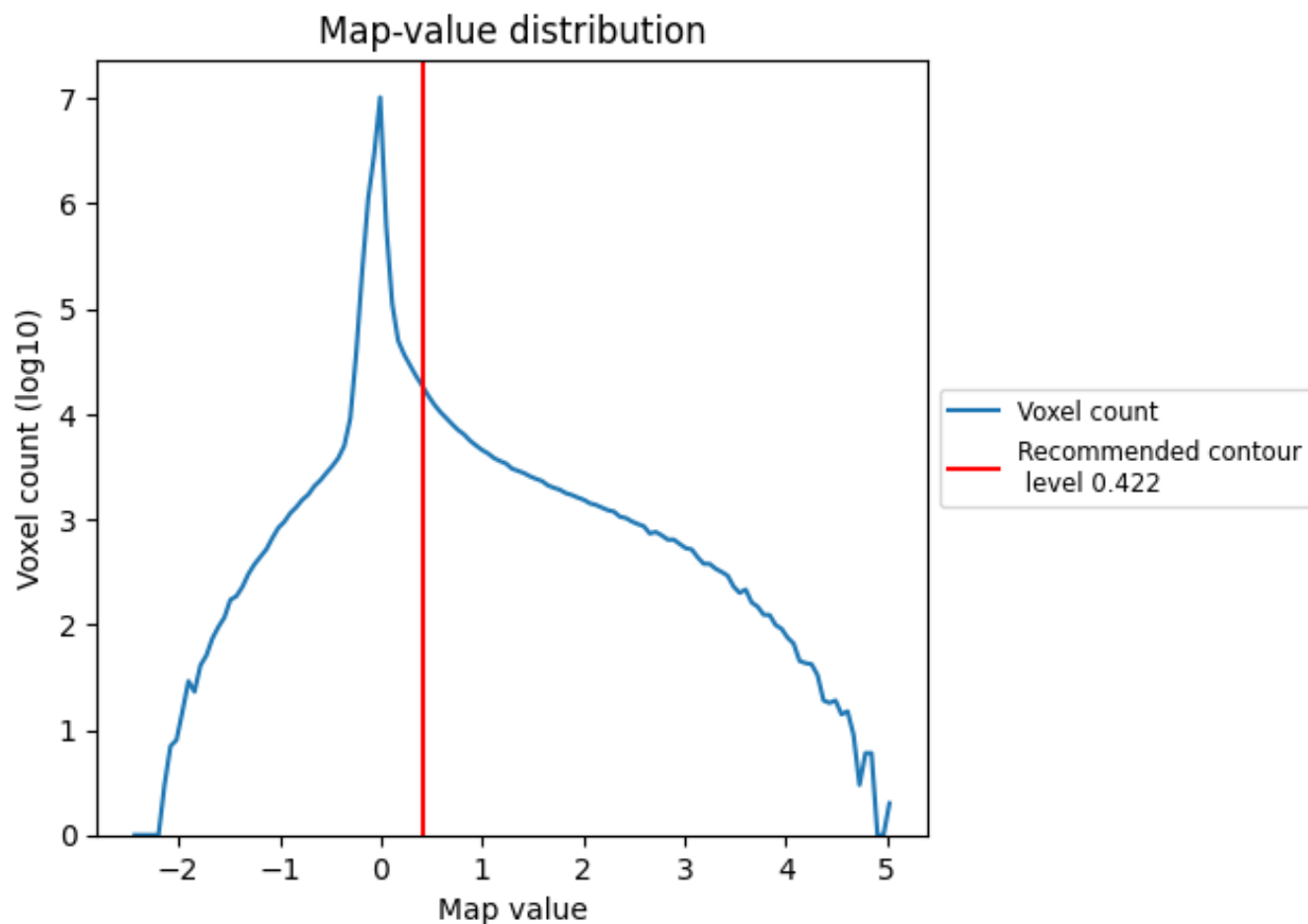
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

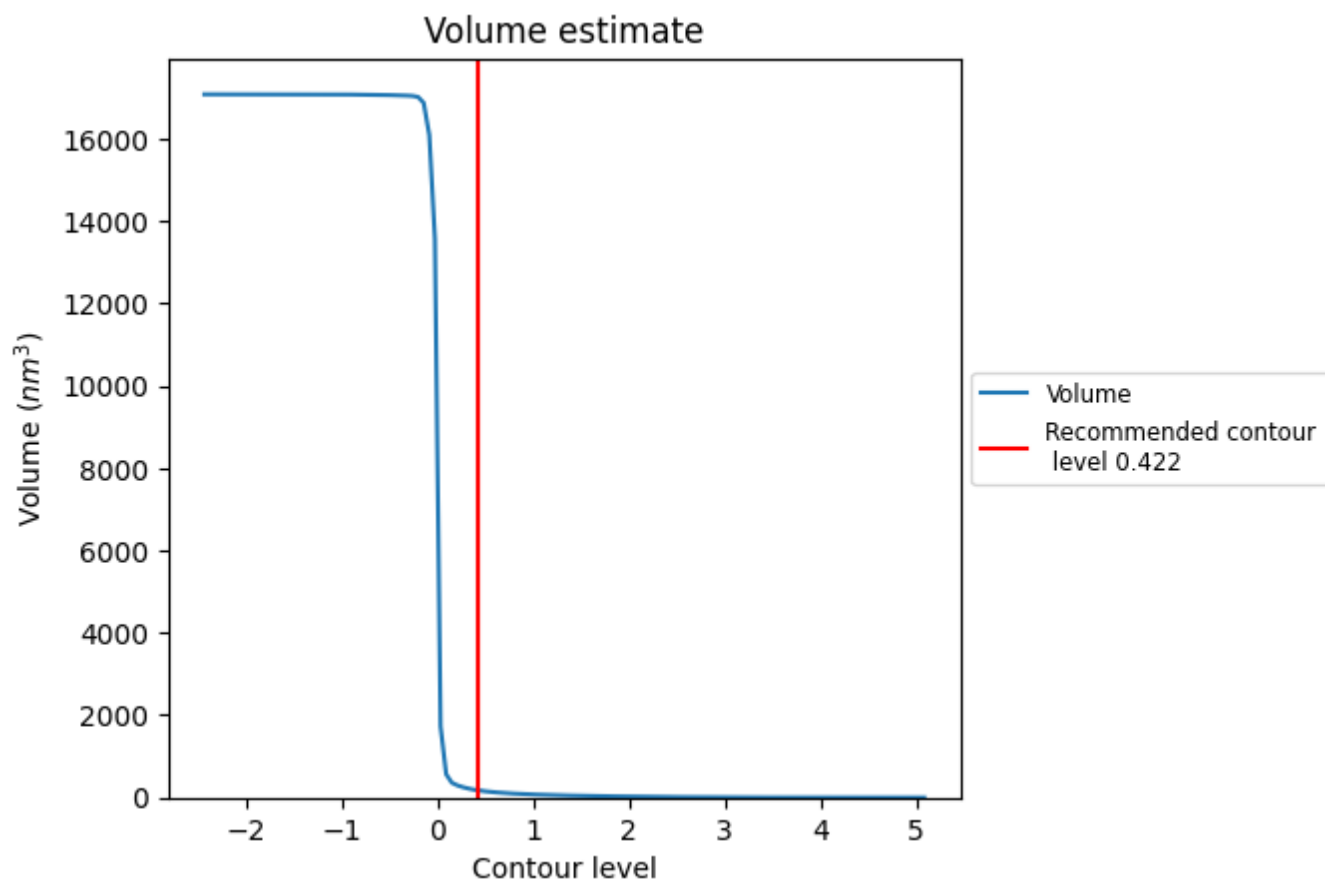
This section contains the results of statistical analysis of the map.

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.

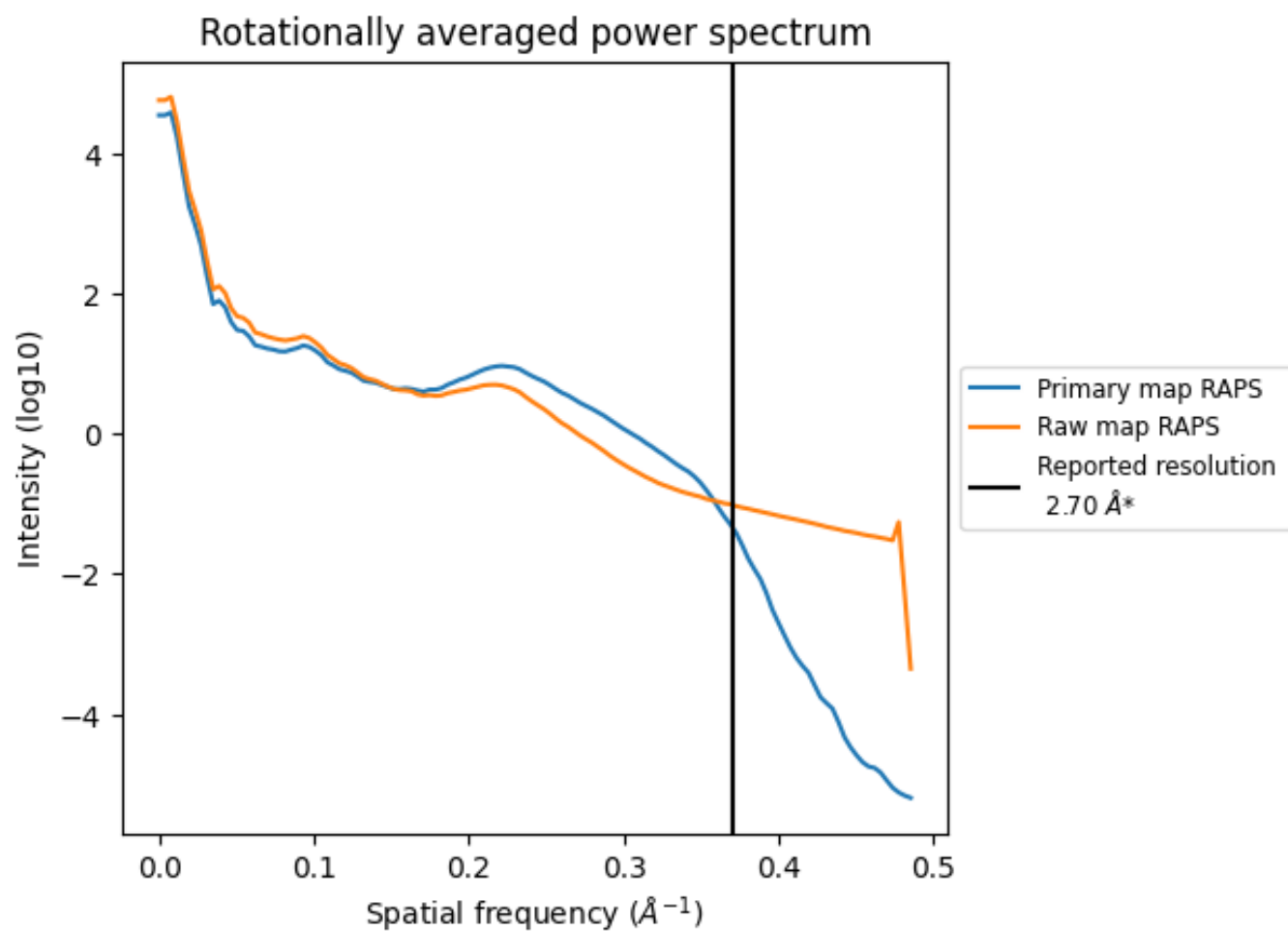
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm^3 ; this corresponds to an approximate mass of 160 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 ⓘ

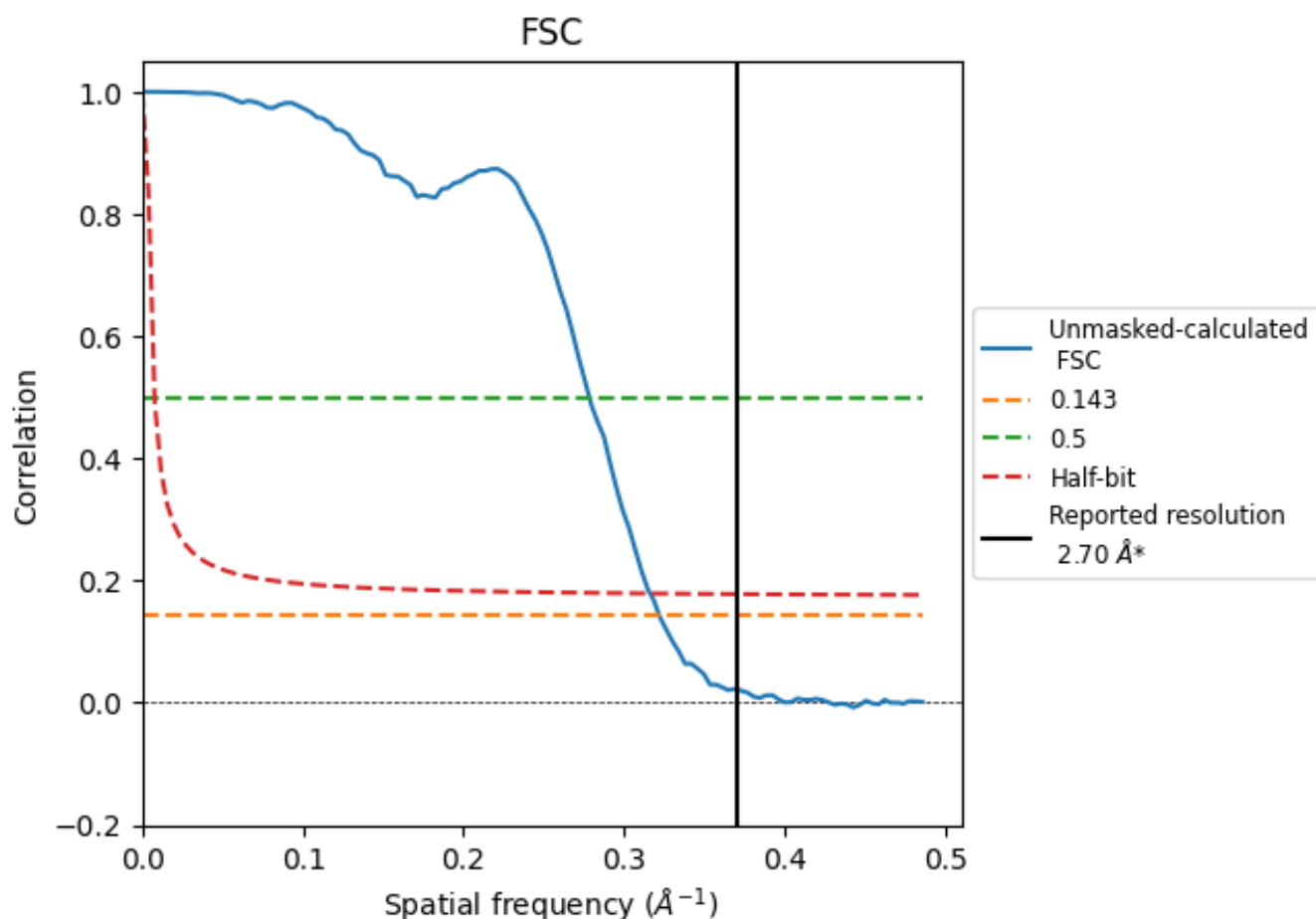


*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

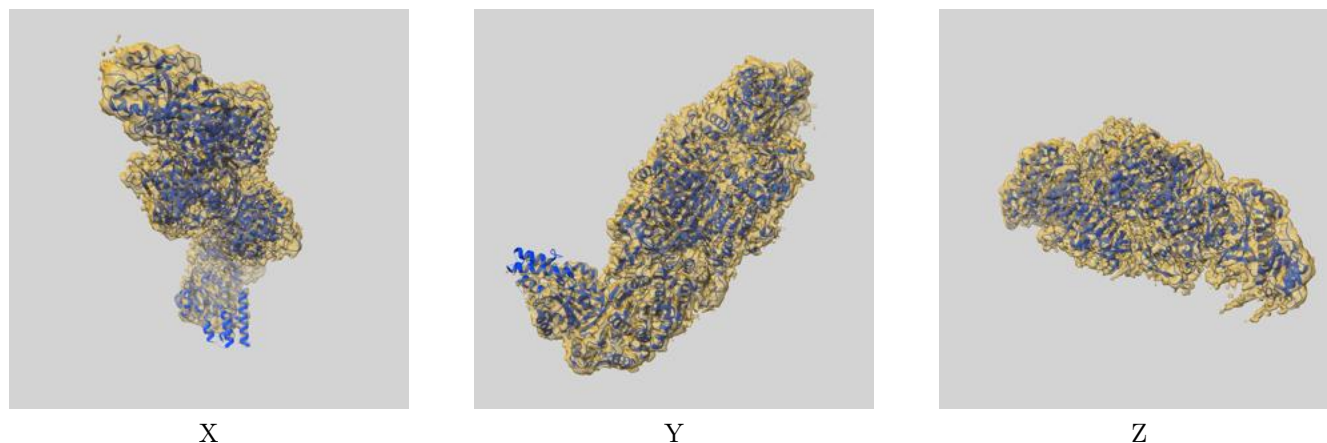
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.59	3.16

*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 3.11 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

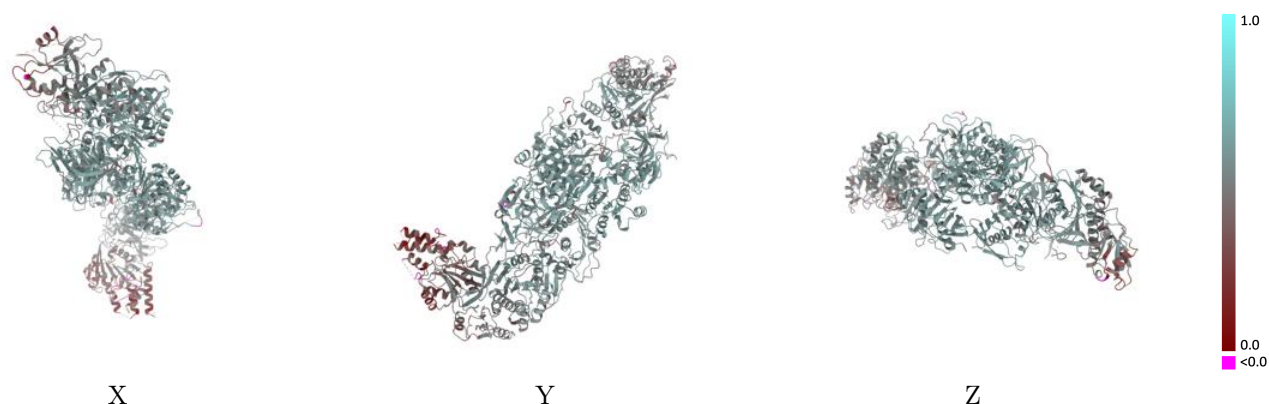
This section contains information regarding the fit between EMDB map EMD-28690 and PDB model 8EYI. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



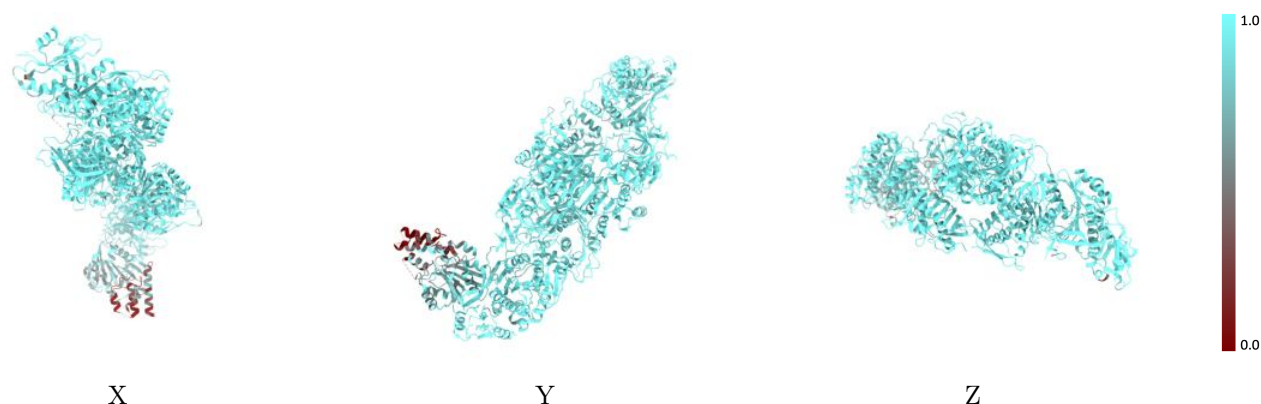
The images above show the 3D surface view of the map at the recommended contour level 0.422 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



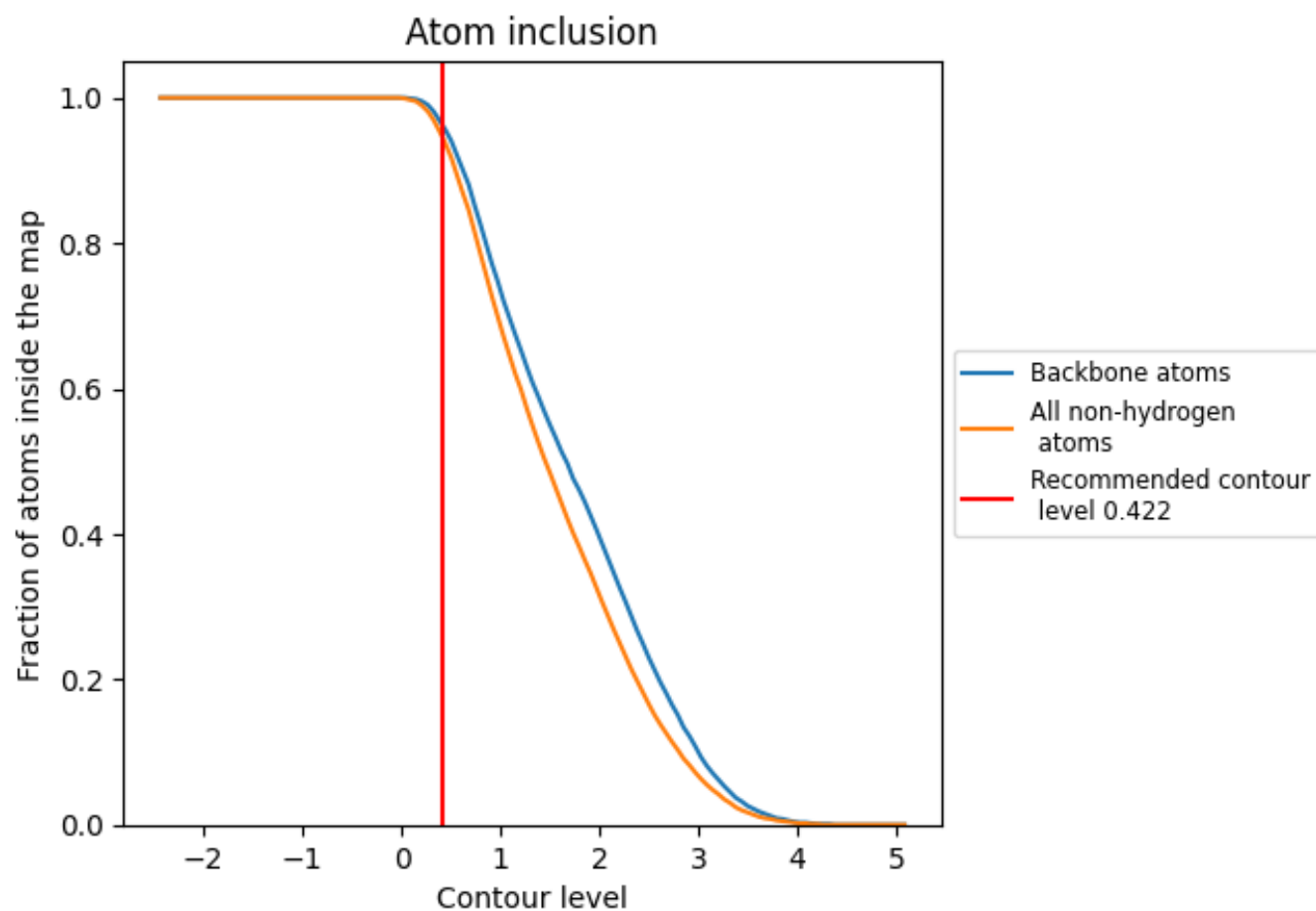
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.422).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.422) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9440	0.5210
E	0.9800	0.5410
F	0.9150	0.5050

