



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 08:42 PM UTC

PDB ID : 9HUX / pdb\_00009hux  
EMDB ID : EMD-52419  
Title : CryoEM map of the large glutamate dehydrogenase composed of 180 kDa subunits from Mycobacterium smegmatis obtained in the presence of NAD<sup>+</sup> and L-glutamate. Open Tetramer.  
Authors : Lazaro, M.; Chamorro, N.; Lopez-Alonso, J.P.; Charro, D.; Rasia, R.M.; Jimenez-Oses, G.; Valle, M.; Lisa, M.N.  
Deposited on : 2024-12-23  
Resolution : 3.88 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](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.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

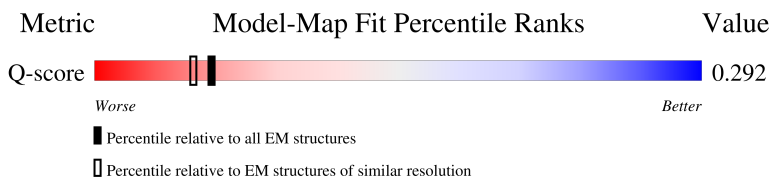
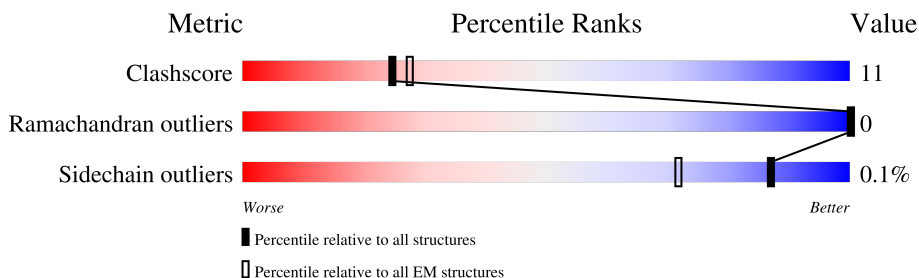
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




The reported resolution of this entry is 3.88 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	8773 ( 3.38 - 4.38 )

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	1611	
1	B	1611	
1	C	1611	

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Mol	Chain	Length	Quality of chain
1	D	1611	 A horizontal bar chart showing the quality of chain D. The bar is divided into three segments: a green segment representing 51%, a yellow segment representing 16%, and a grey segment representing 33%. The percentages are labeled below each segment.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33576 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 NAD-specific glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	B	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	C	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	D	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP A0R1C2
A	-15	HIS	-	expression tag	UNP A0R1C2
A	-14	HIS	-	expression tag	UNP A0R1C2
A	-13	HIS	-	expression tag	UNP A0R1C2
A	-12	HIS	-	expression tag	UNP A0R1C2
A	-11	HIS	-	expression tag	UNP A0R1C2
A	-10	HIS	-	expression tag	UNP A0R1C2
A	-9	GLU	-	expression tag	UNP A0R1C2
A	-8	ASN	-	expression tag	UNP A0R1C2
A	-7	LEU	-	expression tag	UNP A0R1C2
A	-6	TYR	-	expression tag	UNP A0R1C2
A	-5	PHE	-	expression tag	UNP A0R1C2
A	-4	GLN	-	expression tag	UNP A0R1C2
A	-3	GLY	-	expression tag	UNP A0R1C2
A	-2	ALA	-	expression tag	UNP A0R1C2
A	-1	ALA	-	expression tag	UNP A0R1C2
A	0	SER	-	expression tag	UNP A0R1C2
B	-16	MET	-	initiating methionine	UNP A0R1C2
B	-15	HIS	-	expression tag	UNP A0R1C2
B	-14	HIS	-	expression tag	UNP A0R1C2
B	-13	HIS	-	expression tag	UNP A0R1C2
B	-12	HIS	-	expression tag	UNP A0R1C2

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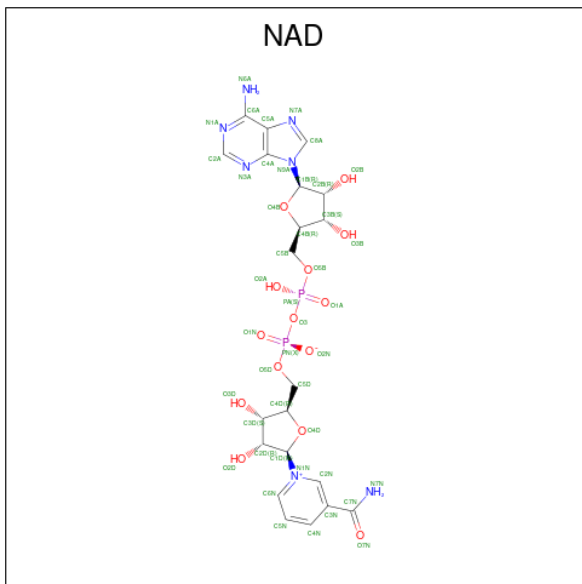
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0R1C2
B	-10	HIS	-	expression tag	UNP A0R1C2
B	-9	GLU	-	expression tag	UNP A0R1C2
B	-8	ASN	-	expression tag	UNP A0R1C2
B	-7	LEU	-	expression tag	UNP A0R1C2
B	-6	TYR	-	expression tag	UNP A0R1C2
B	-5	PHE	-	expression tag	UNP A0R1C2
B	-4	GLN	-	expression tag	UNP A0R1C2
B	-3	GLY	-	expression tag	UNP A0R1C2
B	-2	ALA	-	expression tag	UNP A0R1C2
B	-1	ALA	-	expression tag	UNP A0R1C2
B	0	SER	-	expression tag	UNP A0R1C2
C	-16	MET	-	initiating methionine	UNP A0R1C2
C	-15	HIS	-	expression tag	UNP A0R1C2
C	-14	HIS	-	expression tag	UNP A0R1C2
C	-13	HIS	-	expression tag	UNP A0R1C2
C	-12	HIS	-	expression tag	UNP A0R1C2
C	-11	HIS	-	expression tag	UNP A0R1C2
C	-10	HIS	-	expression tag	UNP A0R1C2
C	-9	GLU	-	expression tag	UNP A0R1C2
C	-8	ASN	-	expression tag	UNP A0R1C2
C	-7	LEU	-	expression tag	UNP A0R1C2
C	-6	TYR	-	expression tag	UNP A0R1C2
C	-5	PHE	-	expression tag	UNP A0R1C2
C	-4	GLN	-	expression tag	UNP A0R1C2
C	-3	GLY	-	expression tag	UNP A0R1C2
C	-2	ALA	-	expression tag	UNP A0R1C2
C	-1	ALA	-	expression tag	UNP A0R1C2
C	0	SER	-	expression tag	UNP A0R1C2
D	-16	MET	-	initiating methionine	UNP A0R1C2
D	-15	HIS	-	expression tag	UNP A0R1C2
D	-14	HIS	-	expression tag	UNP A0R1C2
D	-13	HIS	-	expression tag	UNP A0R1C2
D	-12	HIS	-	expression tag	UNP A0R1C2
D	-11	HIS	-	expression tag	UNP A0R1C2
D	-10	HIS	-	expression tag	UNP A0R1C2
D	-9	GLU	-	expression tag	UNP A0R1C2
D	-8	ASN	-	expression tag	UNP A0R1C2
D	-7	LEU	-	expression tag	UNP A0R1C2
D	-6	TYR	-	expression tag	UNP A0R1C2
D	-5	PHE	-	expression tag	UNP A0R1C2
D	-4	GLN	-	expression tag	UNP A0R1C2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP A0R1C2
D	-2	ALA	-	expression tag	UNP A0R1C2
D	-1	ALA	-	expression tag	UNP A0R1C2
D	0	SER	-	expression tag	UNP A0R1C2

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0



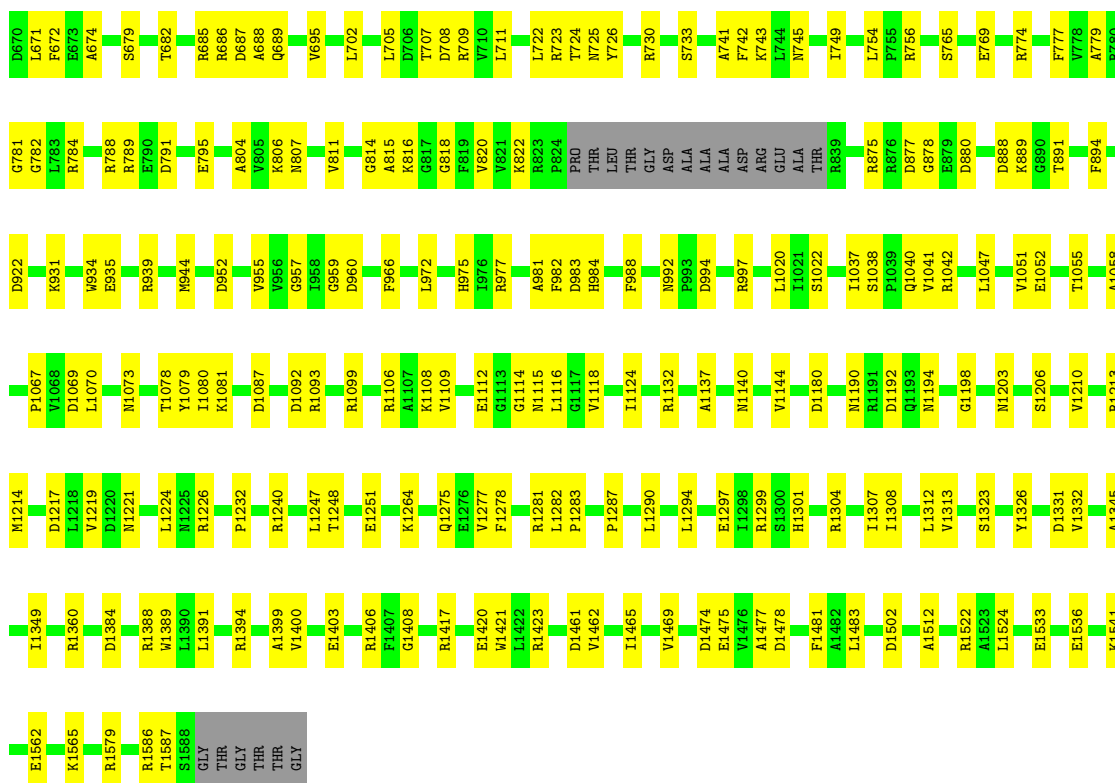




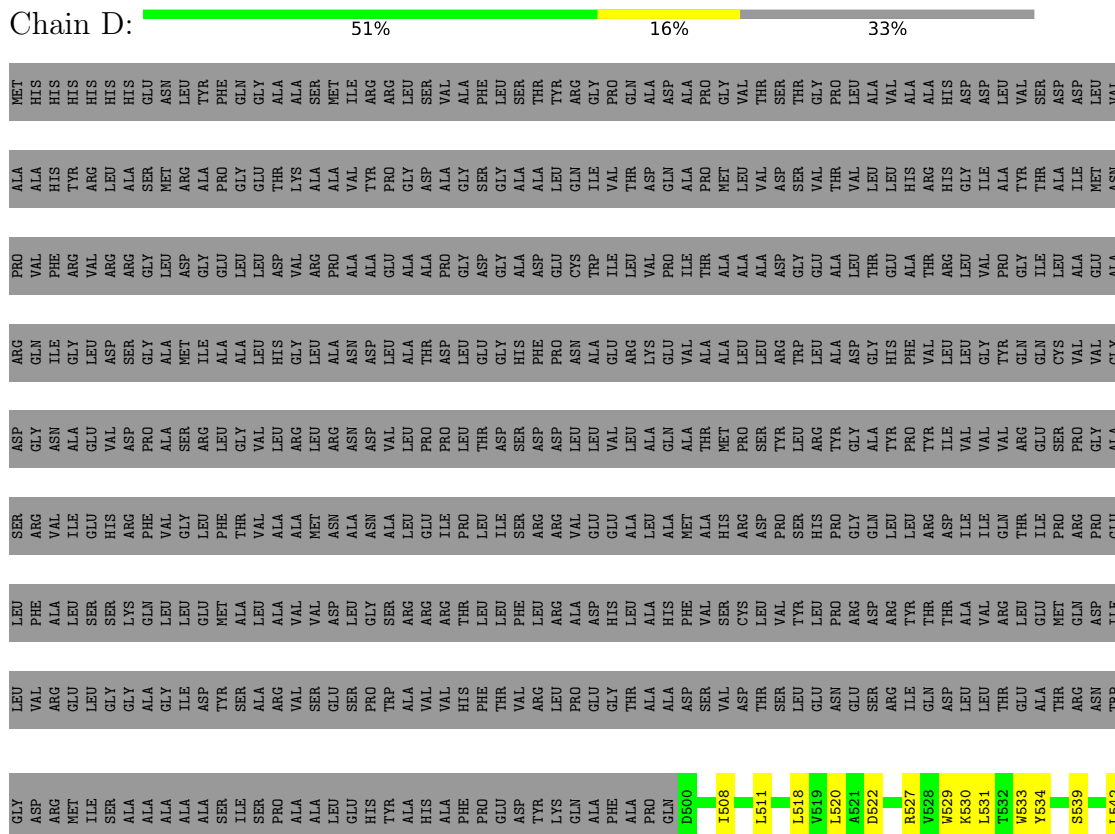


Category	Percentage
Very good	51%
Good	16%
Not good	33%





- Molecule 1: NAD-specific glutamate dehydrogenase



E1539	L546	S656	V778	D1069	D1217	I1349	E1539
E1540	L547	V657	A779	L1070	L1218	R1360	E1540
K1541	G553	T664	R784	N1073	V1219	L1377	K1541
I1542	V554	T665	R788	Y1079	N1221	D1384	I1542
E1562	V555	T669	R789	I1080	N1224	R1388	E1562
K1565	V556	D670	E790	K1081	L1225	W1389	K1565
R1579	L557	L671	D791	D1087	R1226	L1390	R1579
R1586	E558	F672	E795	D1092	P1232	L1391	R1586
T1587	E559	F673	A674	R1093	R1240	L1392	T1587
S1588	R560	A674	A804	R1099	G1246	Y1393	S1588
GLY	T563	R685	G857	R1106	L1247	R1394	GLY
THR	L564	R686	R806	A1107	T1248	A1399	THR
GLY	R566	D687	N807	K1108	E1251	V1400	GLY
THR	R566	A688	V811	V1109	K1284	E1403	THR
THR	L570	Q689	G814	E1112	Q1275	R1406	THR
GLY	W573	V685	A815	G1113	E1276	F1407	GLY
	I574	L702	V820	N1114	V1277	G1408	
	Y575	L705	K822	N1115	F1278	V1421	
	Q576	D706	R823	L1116	R1281	L1422	
I579	S580	T707	P824	G1117	L1282	R1423	I579
S580	P581	R708	PRO	V1118	P1283	D1461	S580
H582	V710	R709	THR	I1124	P1287	V1462	H582
I585	L711	L711	LEU	R1132	L1294	I1465	I585
P586	L722	L722	THR	A1137	E1297	V1469	P586
H587	R723	R723	GLY	N1140	I1298	D1474	H587
A604	T724	T724	ASP	V1144	I1299	E1475	A604
A607	N725	N725	ALA	D1180	S1300	V1476	A607
I608	Y726	Y726	ALA	N1190	H1301	D1478	I608
	R730	R730	ASP	R1191	R1304	F1481	
R612	S733	S733	ARG	D1192	I1307	A1482	R612
D616	A741	A741	GLU	Q1193	I1308	L1483	D616
R617	F742	F742	THR	N1194	L1312	R1501	R617
L621	L744	L744	R839	G1198	V1313	R1510	L621
R624	N745	N745	R875	N1203	S1323	L1511	R624
Q630	I749	I749	R876	S1206	Y1326	A1512	Q630
Q631	L754	L754	D877	L1207	S1209	R1522	Q631
V634	F755	F755	G878	V1210	D1331	L1524	V634
L635	R756	R756	D880	R1213	V1332	E1533	L635
R636	T891	T891	K888	M1214	A1345	E1536	R636
K640	S765	S765	K889				K640
Y649	E769	E769	T891				Y649
S650	R774	R774	F894				S650
Q651	F777	F777	D922				Q651
			K931				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37641	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	439.41602, 439.41602, 439.41602	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2924, 1.2924, 1.2924	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: NAD

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	0.07	0/8502	0.20	0/11541
1	B	0.07	0/8502	0.20	0/11541
1	C	0.07	0/8502	0.20	0/11541
1	D	0.07	0/8502	0.20	0/11541
All	All	0.07	0/34008	0.20	0/46164

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	8350	0	8301	182	0
1	B	8350	0	8301	183	0
1	C	8350	0	8301	179	0
1	D	8350	0	8301	177	0
2	A	44	0	26	6	0
2	B	44	0	26	7	0
2	C	44	0	26	7	0
2	D	44	0	26	7	0
All	All	33576	0	33308	710	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 710 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:960:ASP:HB2	1:B:983:ASP:OD2	1.48	1.14
1:D:960:ASP:HB2	1:D:983:ASP:OD2	1.48	1.14
1:A:960:ASP:HB2	1:A:983:ASP:OD2	1.48	1.13
1:C:960:ASP:HB2	1:C:983:ASP:OD2	1.48	1.13
1:B:960:ASP:CB	1:B:983:ASP:OD2	2.25	0.85

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	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
1	B	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
1	C	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
1	D	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
All	All	4284/6444 (66%)	4164 (97%)	120 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	877/1294 (68%)	876 (100%)	1 (0%)	88	89
1	B	877/1294 (68%)	876 (100%)	1 (0%)	88	89
1	C	877/1294 (68%)	876 (100%)	1 (0%)	88	89
1	D	877/1294 (68%)	876 (100%)	1 (0%)	88	89
All	All	3508/5176 (68%)	3504 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1051	VAL
1	B	1051	VAL
1	C	1051	VAL
1	D	1051	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1190	ASN
1	D	807	ASN
1	C	1295	HIS
1	D	644	GLN
1	D	1115	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	NAD	B	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.58	0
2	NAD	C	1601	-	46,48,48	0.63	1 (2%)	64,73,73	0.59	1 (1%)
2	NAD	A	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.58	0
2	NAD	D	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	C	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	A	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	D	1601	-	-	1/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	NAD	C2N-N1N	2.84	1.38	1.35
2	B	1601	NAD	C2N-N1N	2.84	1.38	1.35
2	D	1601	NAD	C2N-N1N	2.80	1.38	1.35
2	C	1601	NAD	C2N-N1N	2.77	1.38	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1601	NAD	C6N-N1N-C2N	-2.04	120.14	121.88

There are no chirality outliers.

All (4) torsion outliers are listed below:



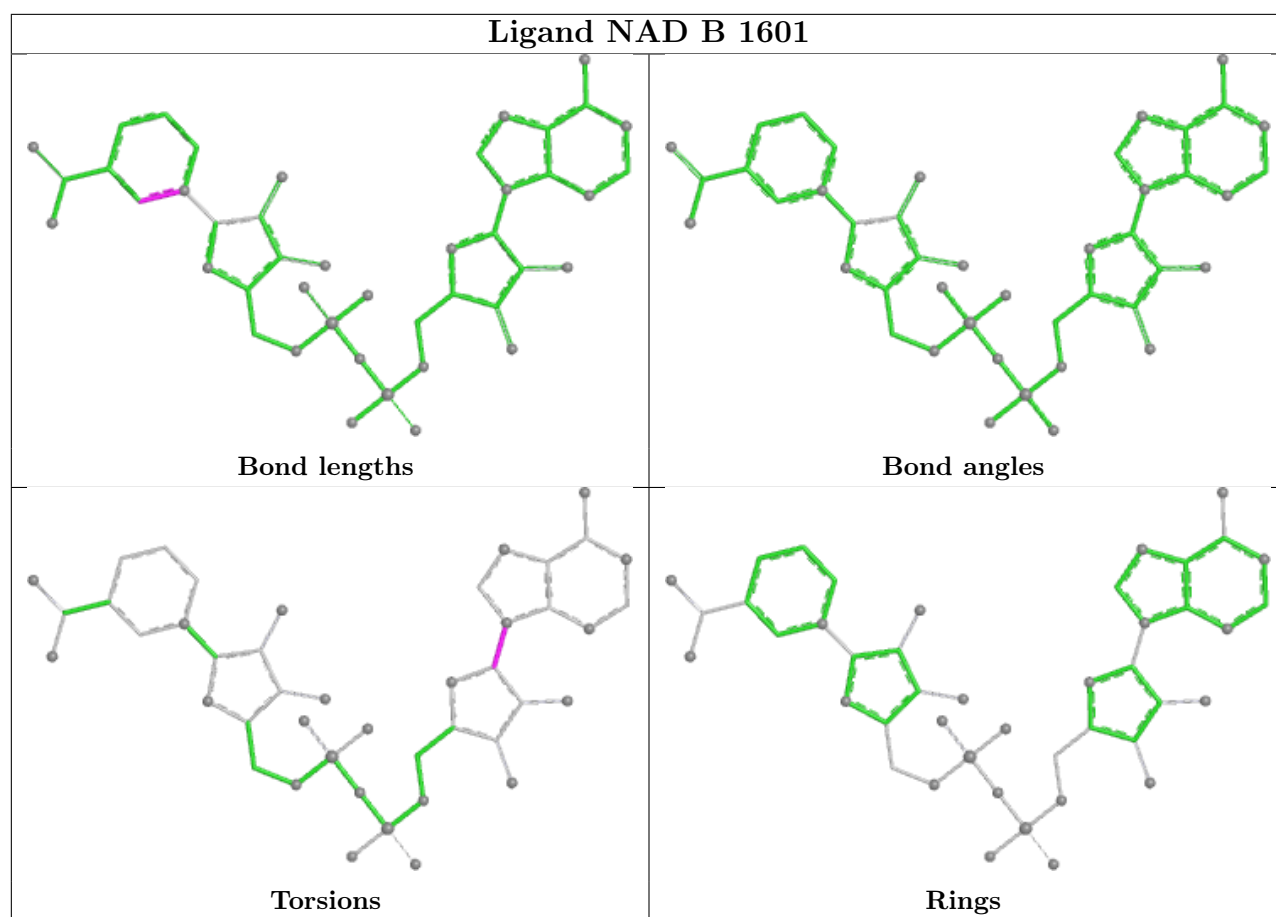
Mol	Chain	Res	Type	Atoms
2	A	1601	NAD	C2B-C1B-N9A-C8A
2	B	1601	NAD	C2B-C1B-N9A-C8A
2	C	1601	NAD	C2B-C1B-N9A-C8A
2	D	1601	NAD	C2B-C1B-N9A-C8A

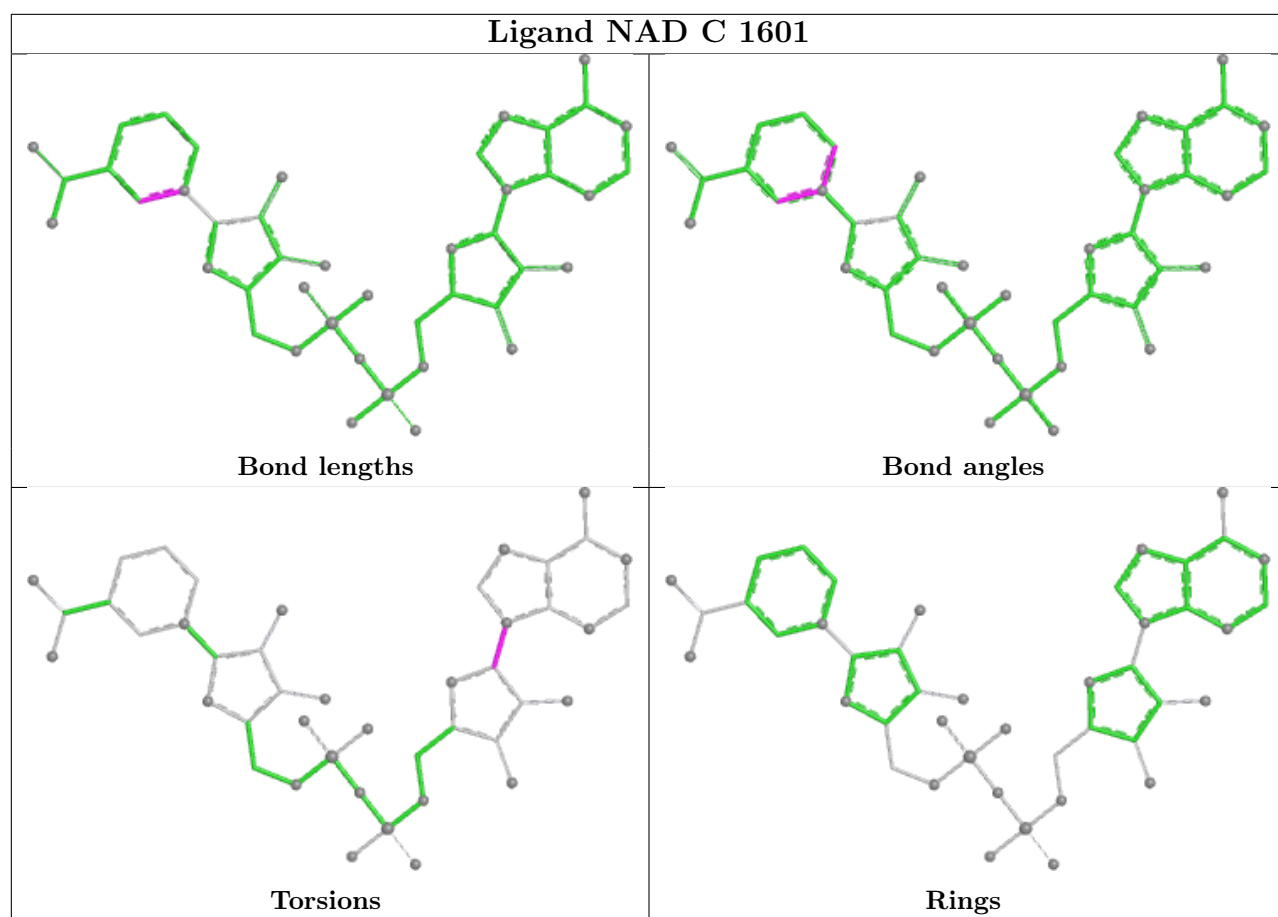
There are no ring outliers.

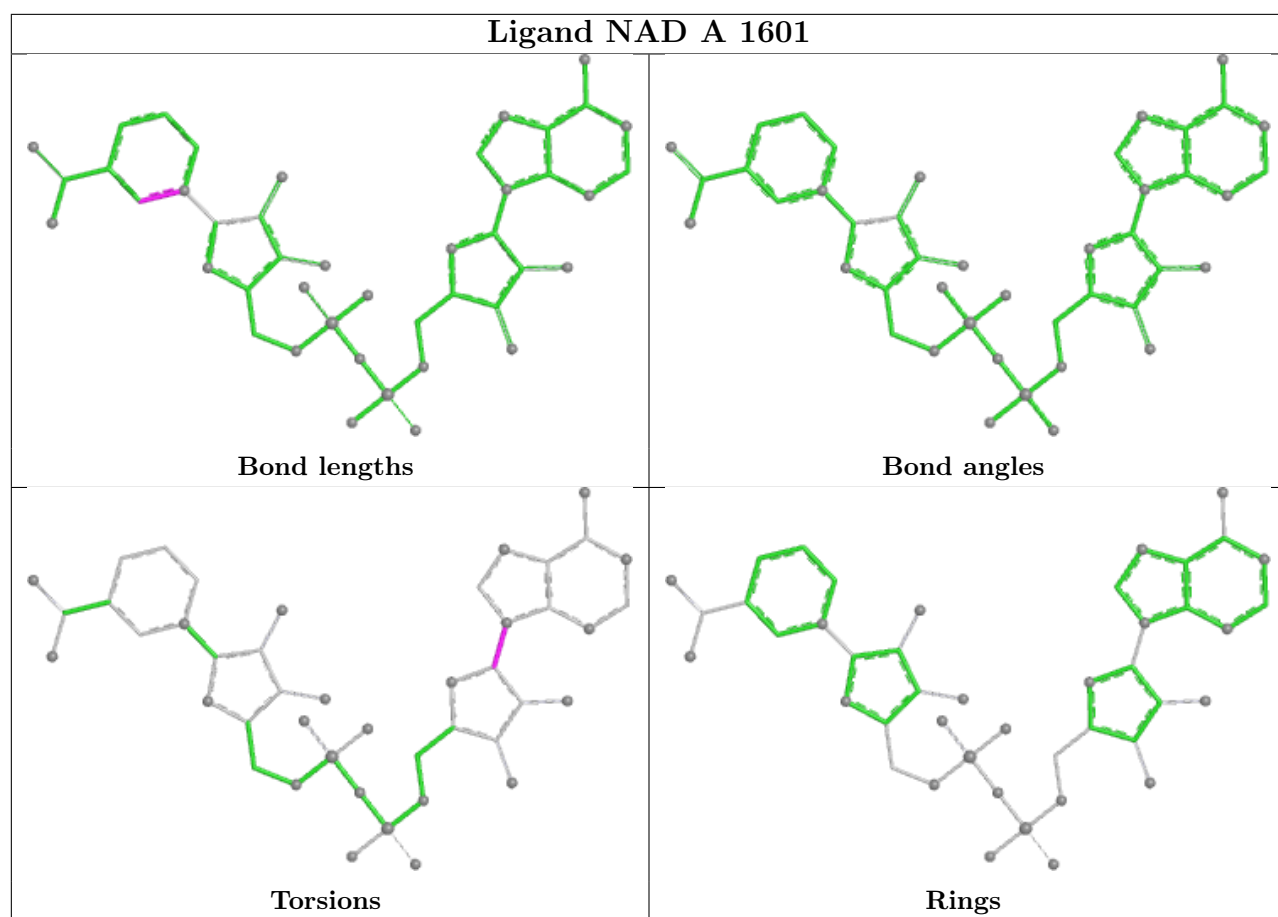
4 monomers are involved in 27 short contacts:

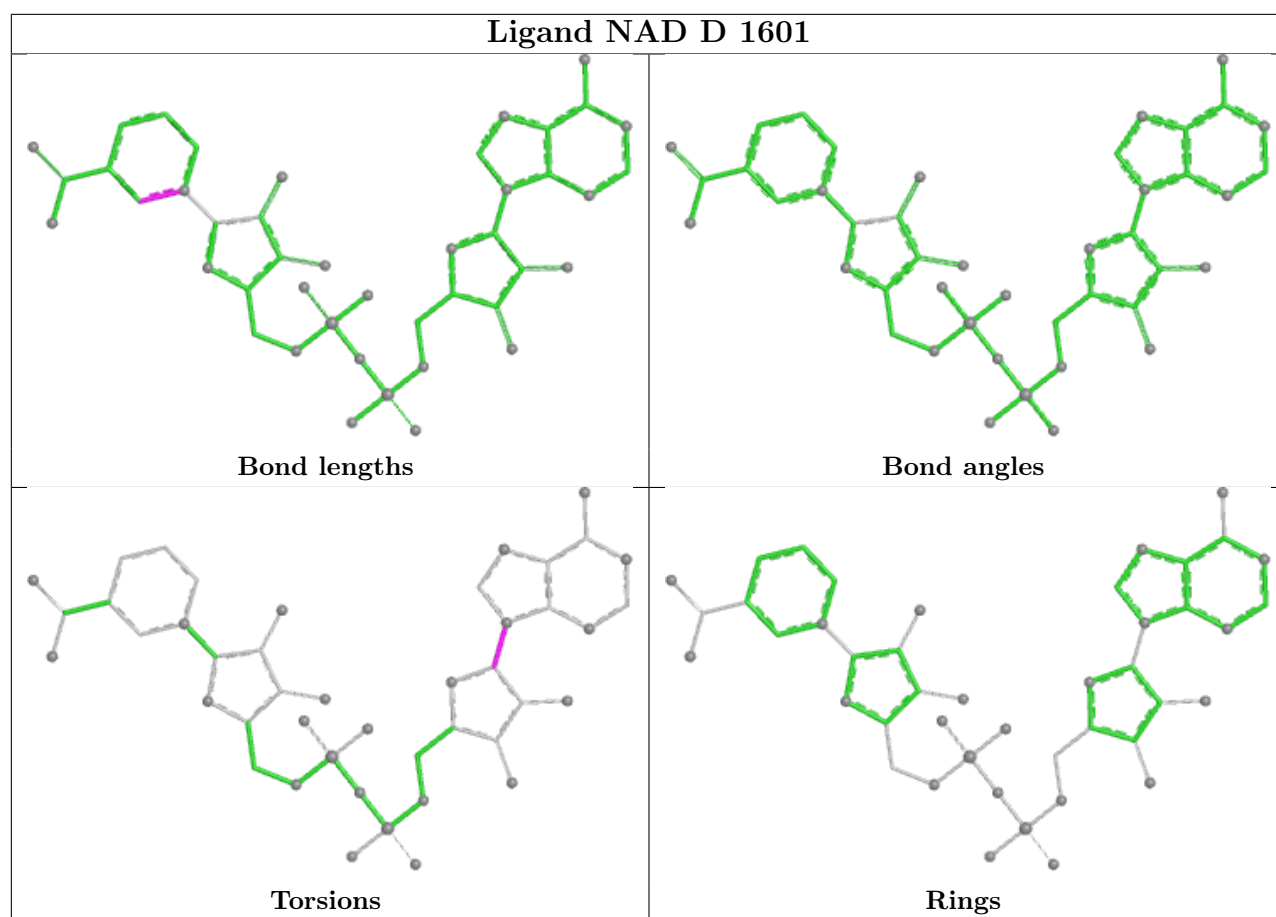
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1601	NAD	7	0
2	C	1601	NAD	7	0
2	A	1601	NAD	6	0
2	D	1601	NAD	7	0

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.

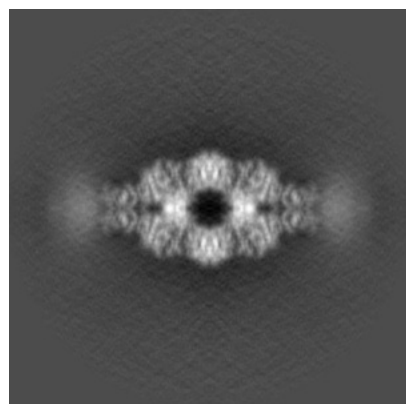
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52419. These allow visual inspection of the internal detail of the map and identification of artifacts.

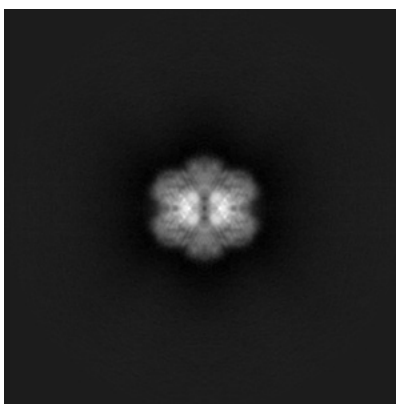
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

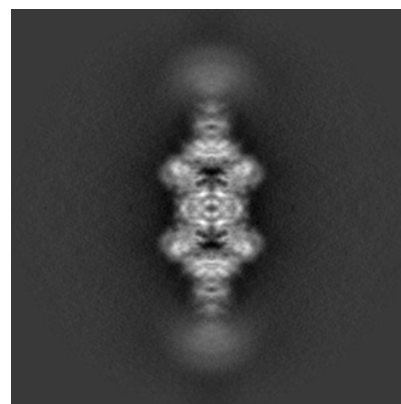
#### 6.1.1 Primary map



X

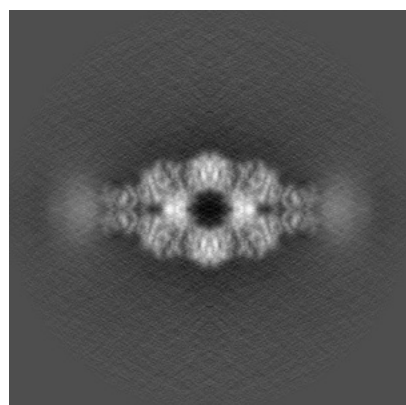


Y

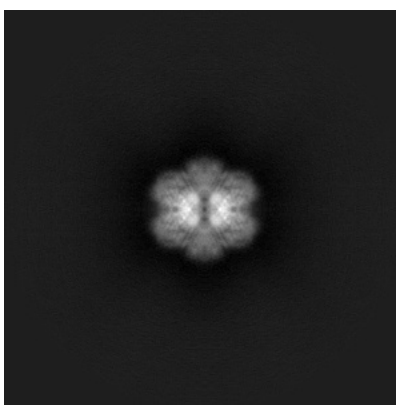


Z

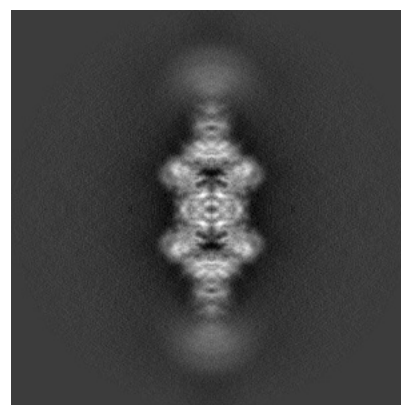
#### 6.1.2 Raw map



X



Y

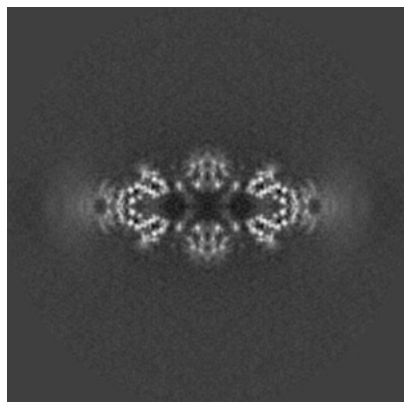


Z

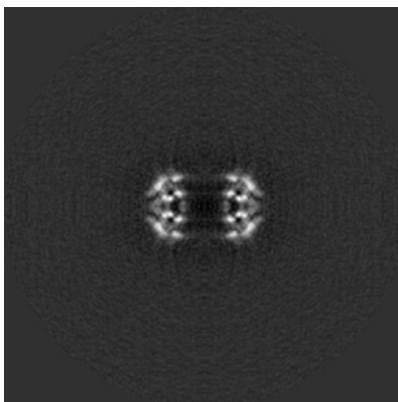
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

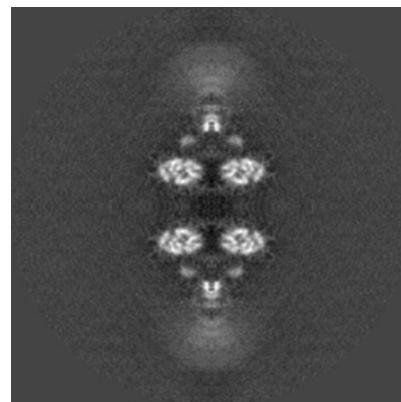
### 6.2.1 Primary map



X Index: 170

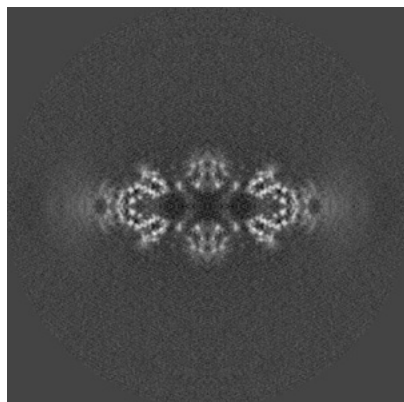


Y Index: 170

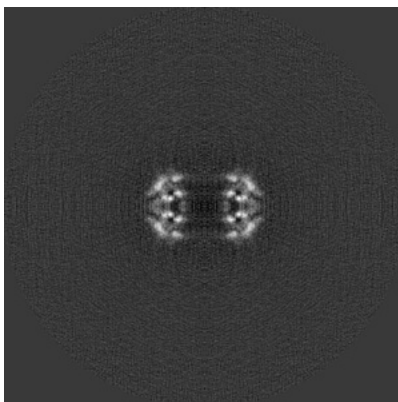


Z Index: 170

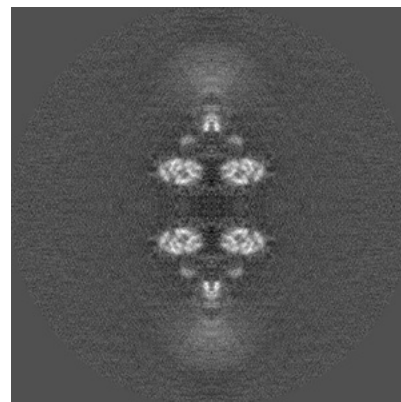
### 6.2.2 Raw map



X Index: 170



Y Index: 170

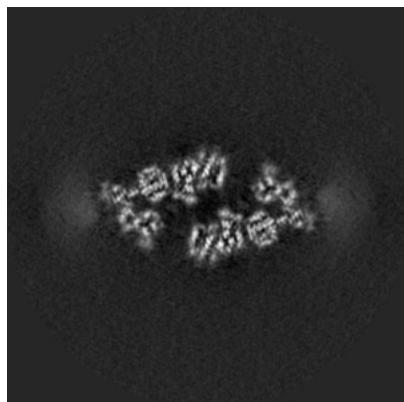


Z Index: 170

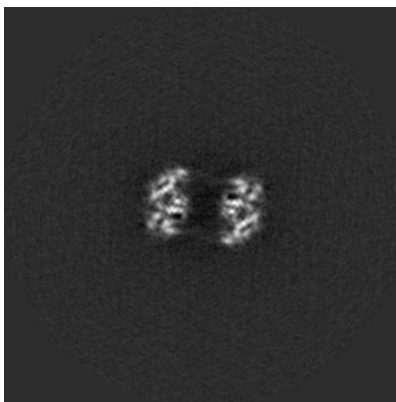
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

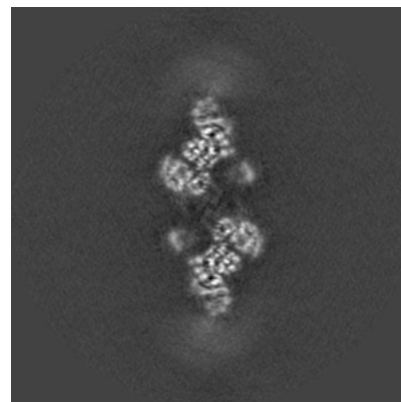
### 6.3.1 Primary map



X Index: 163

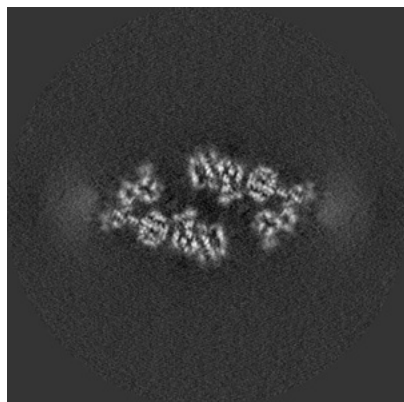


Y Index: 165

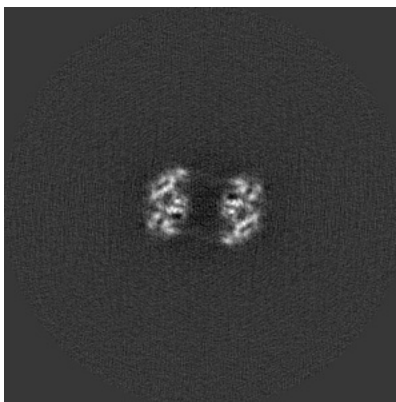


Z Index: 158

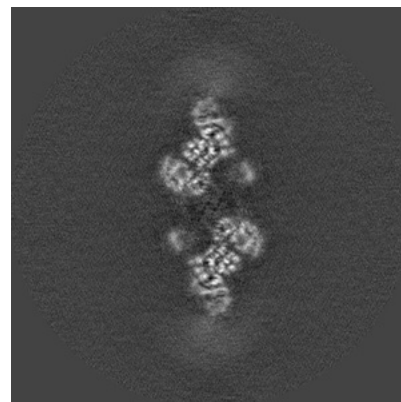
### 6.3.2 Raw map



X Index: 177



Y Index: 165



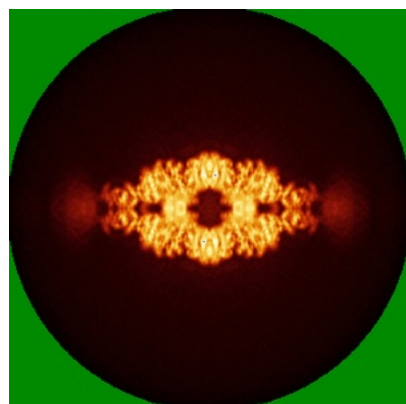
Z Index: 158

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

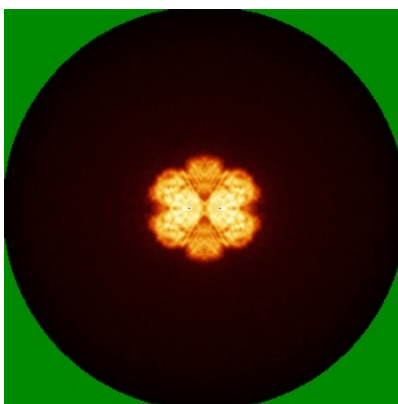


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

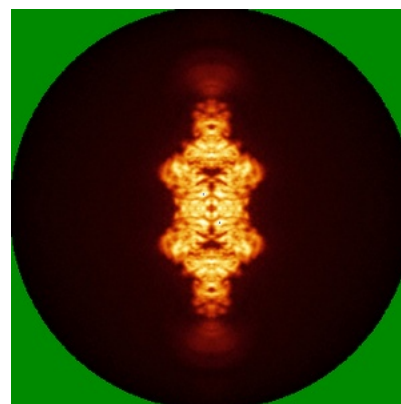
### 6.4.1 Primary map



X

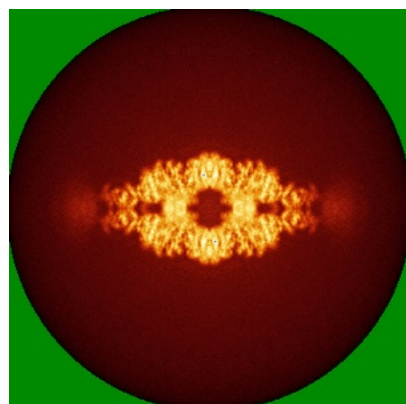


Y

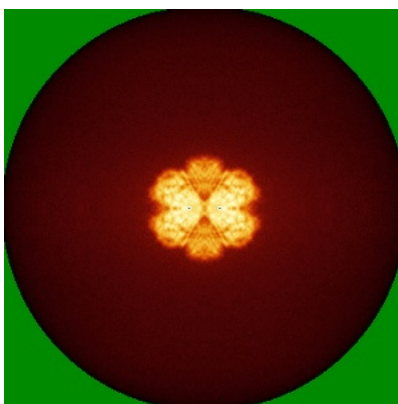


Z

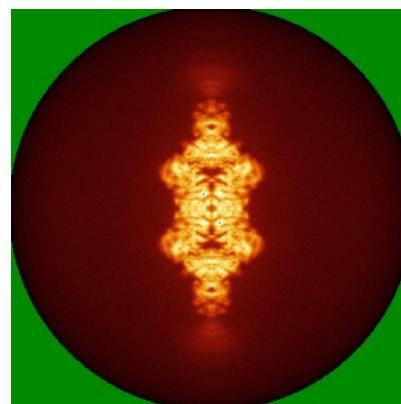
### 6.4.2 Raw map



X



Y

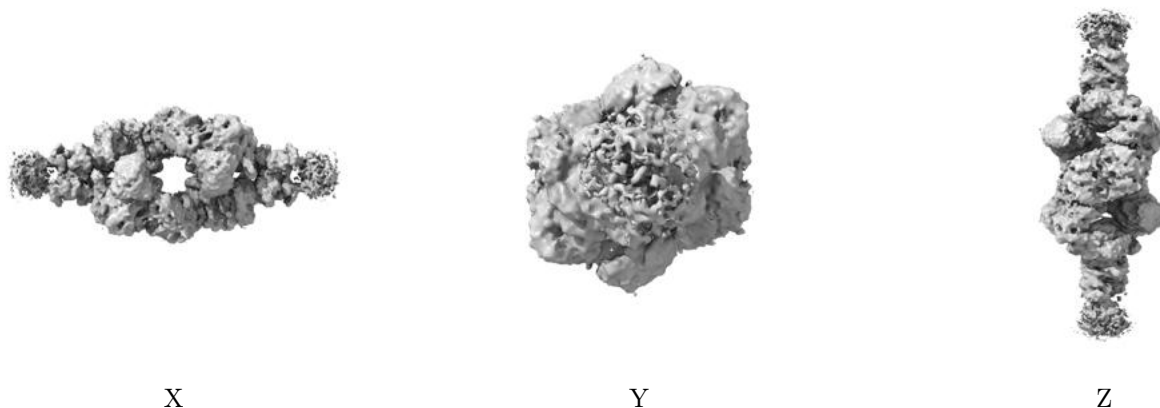


Z

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.

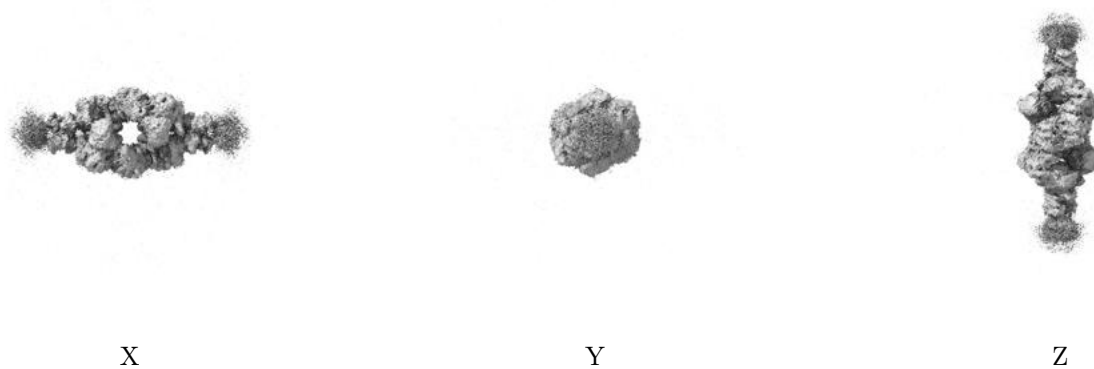
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

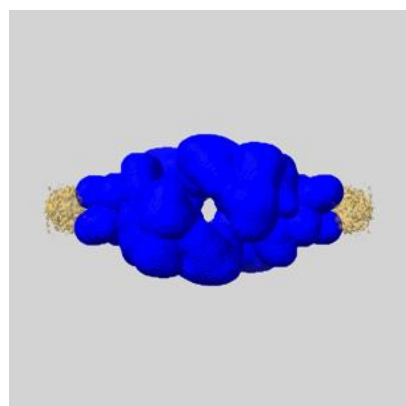
## 6.6 Mask visualisation [i](#)

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

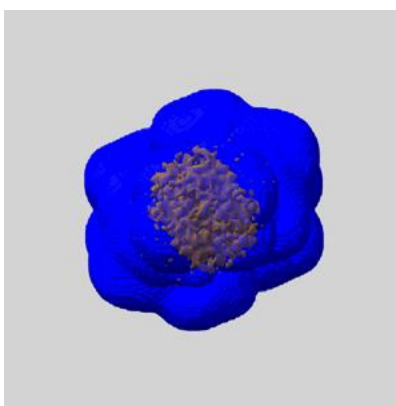
A mask typically either:

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

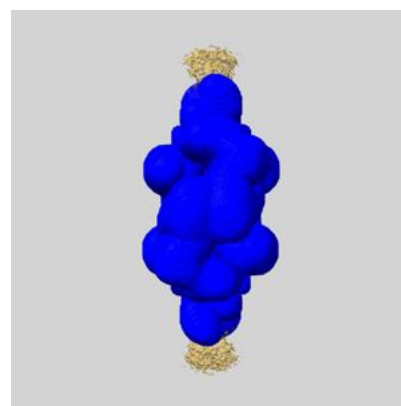
### 6.6.1 emd\_52419\_msk\_1.map [i](#)



X



Y

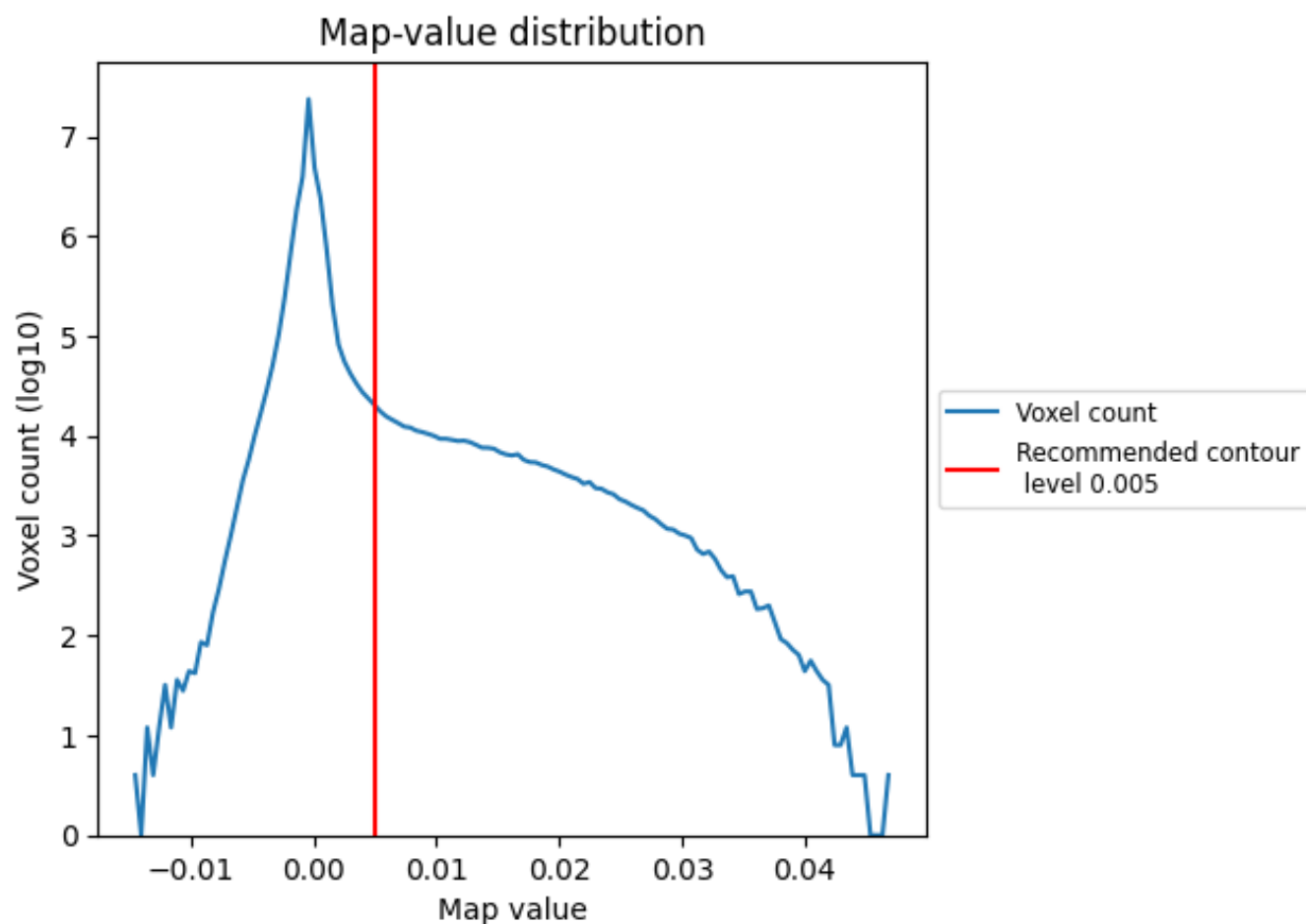


Z

## 7 Map analysis [i](#)

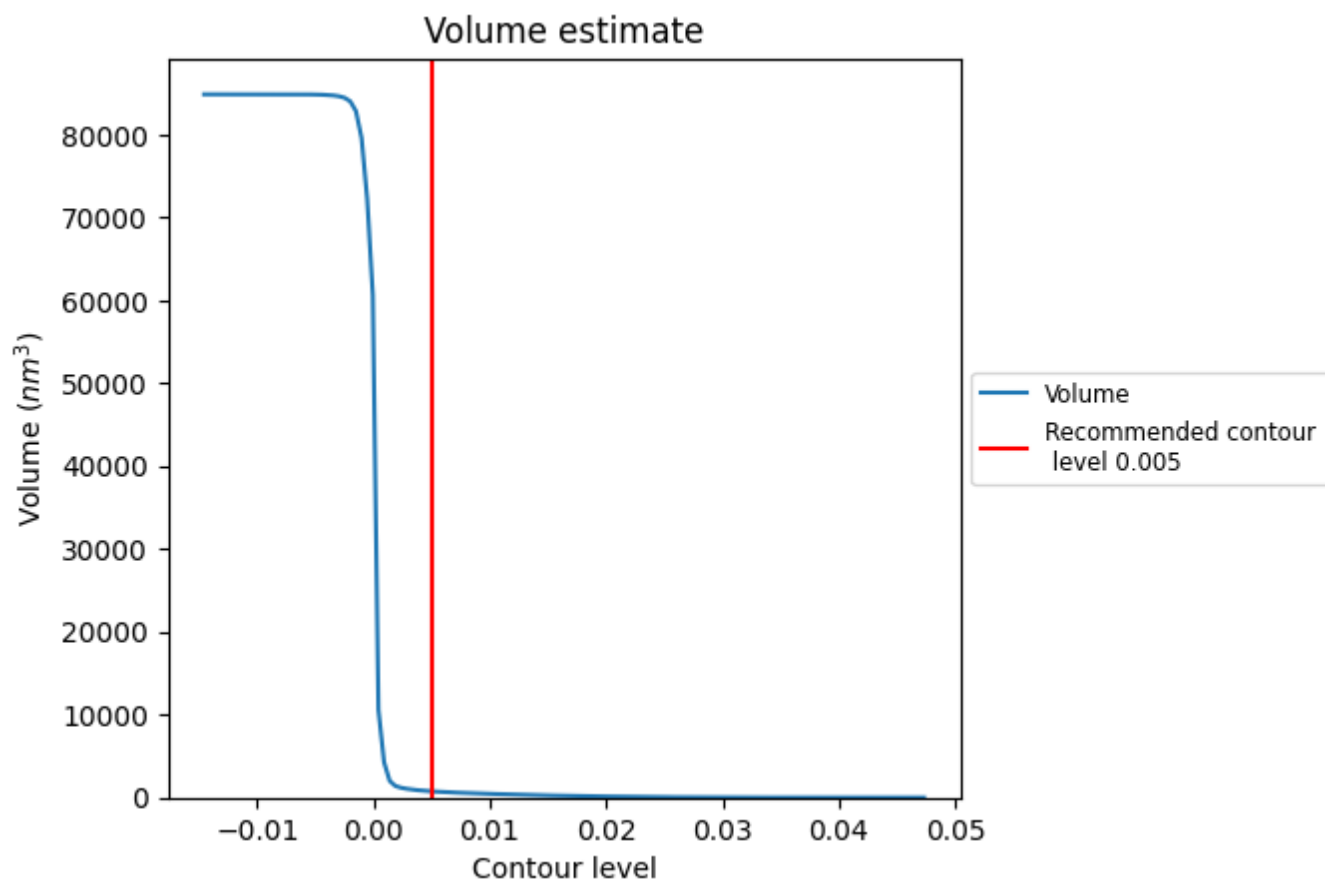
This section contains the results of statistical analysis of the map.

### 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.

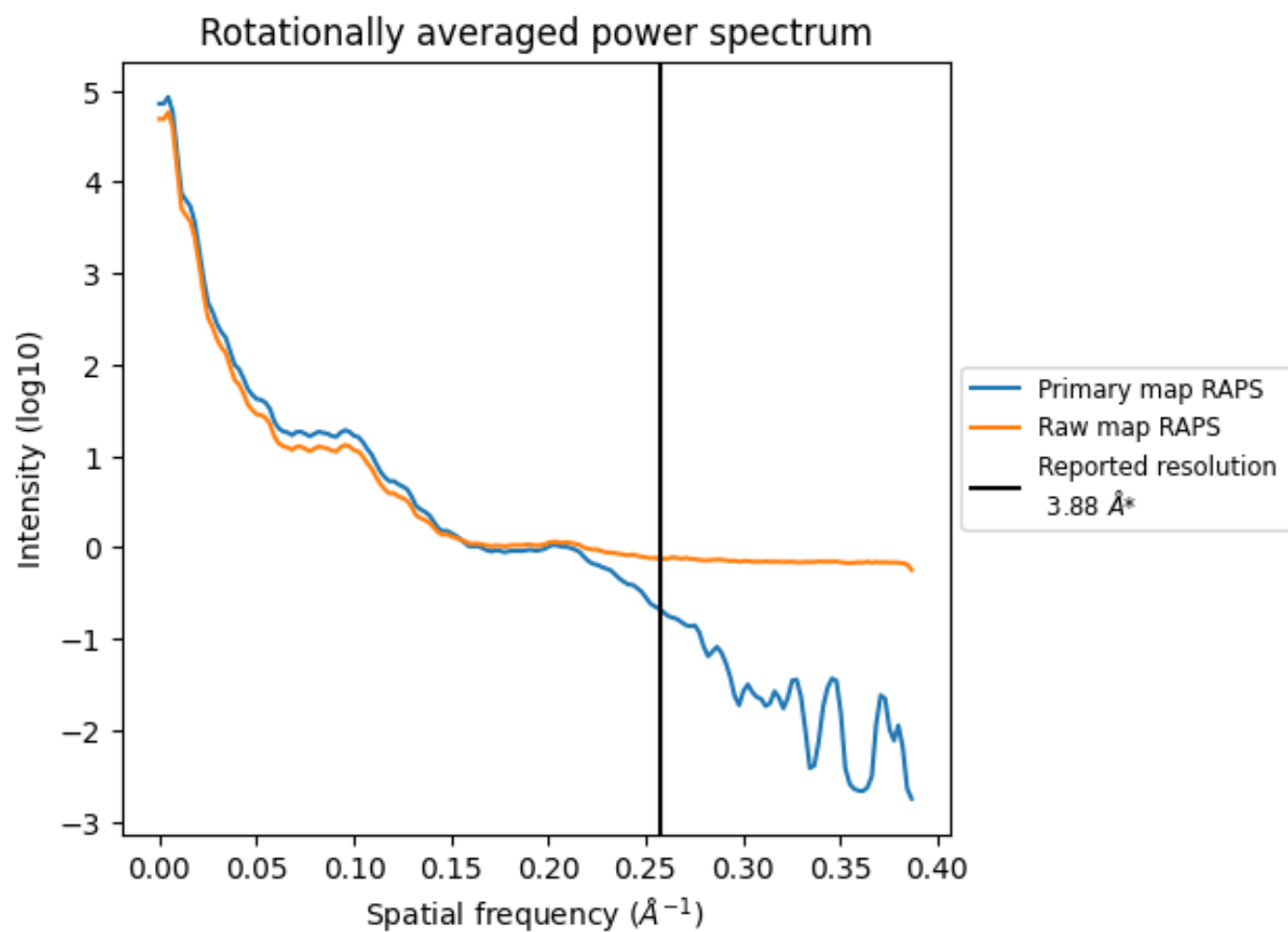
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 751  $\text{nm}^3$ ; this corresponds to an approximate mass of 679 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 ⓘ

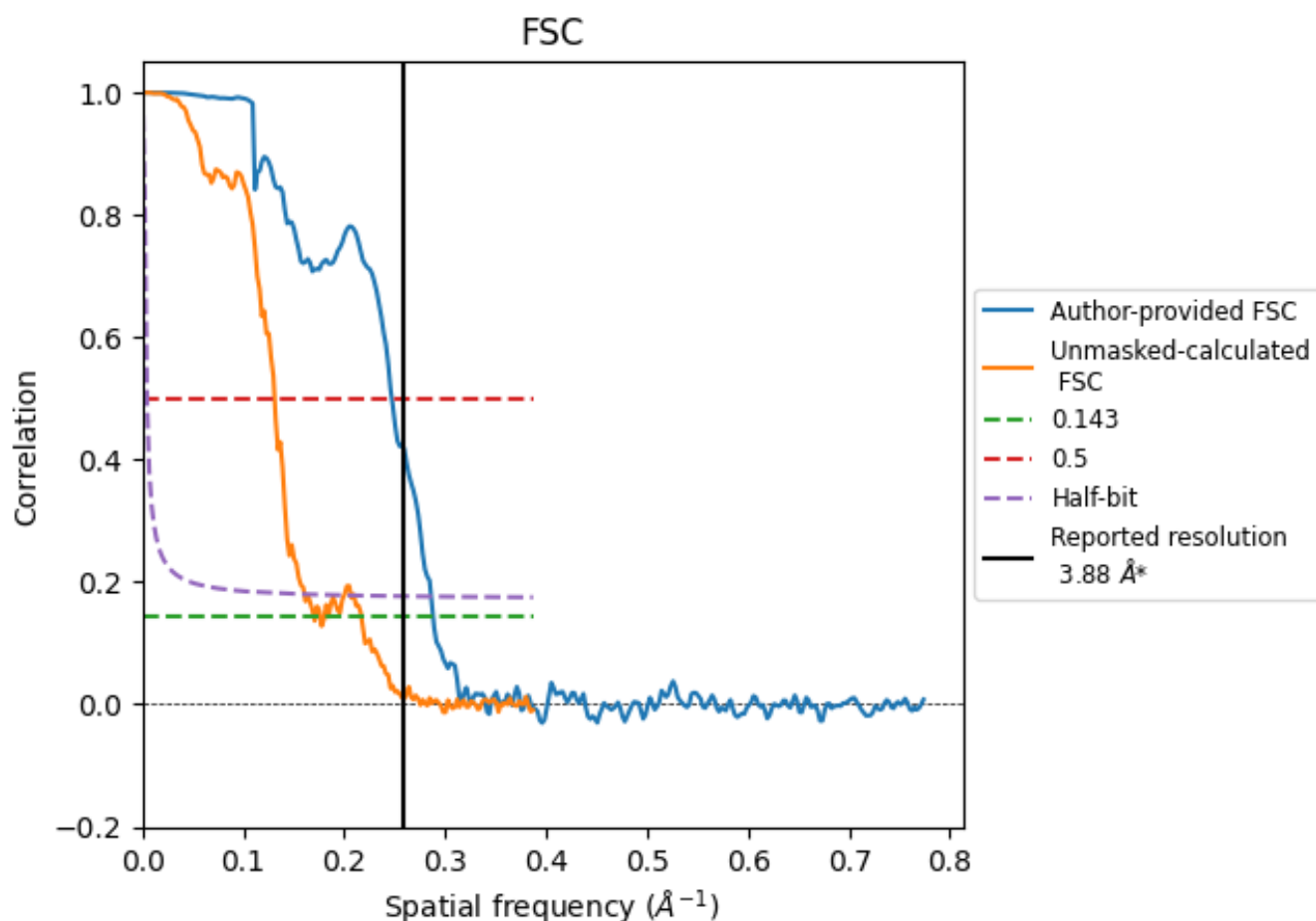


\*Reported resolution corresponds to spatial frequency of 0.258 Å<sup>-1</sup>

## 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  $0.258 \text{ \AA}^{-1}$

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.88	-	-
Author-provided FSC curve	3.47	4.05	3.50
Unmasked-calculated*	5.89	7.64	6.23

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 3.88 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.89 differs from the reported value 3.88 by more than 10 %



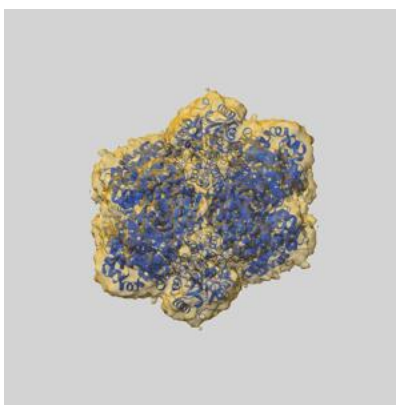
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52419 and PDB model 9HUX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

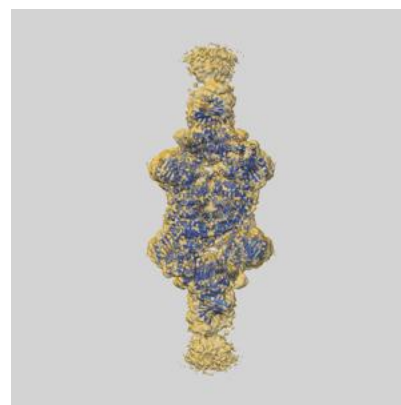
### 9.1 Map-model overlay [i](#)



X



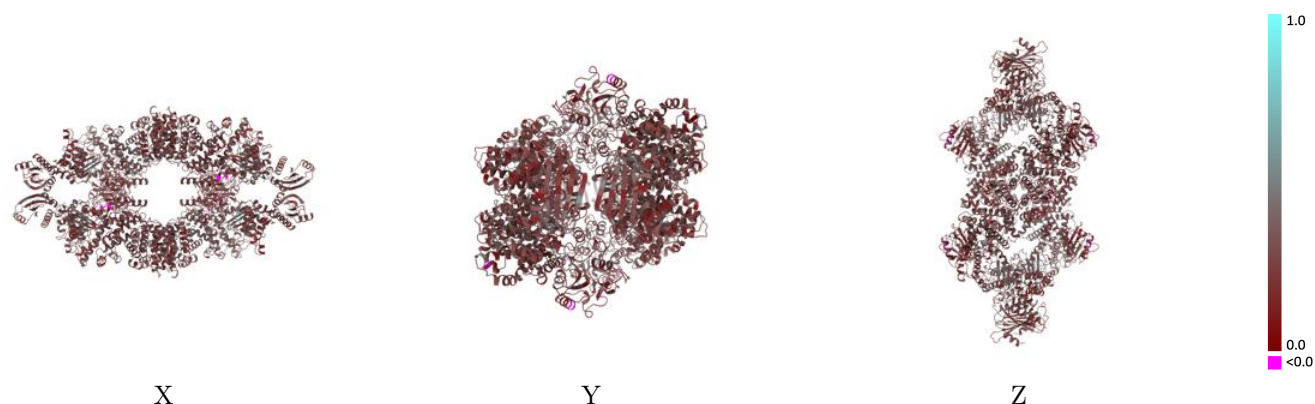
Y



Z

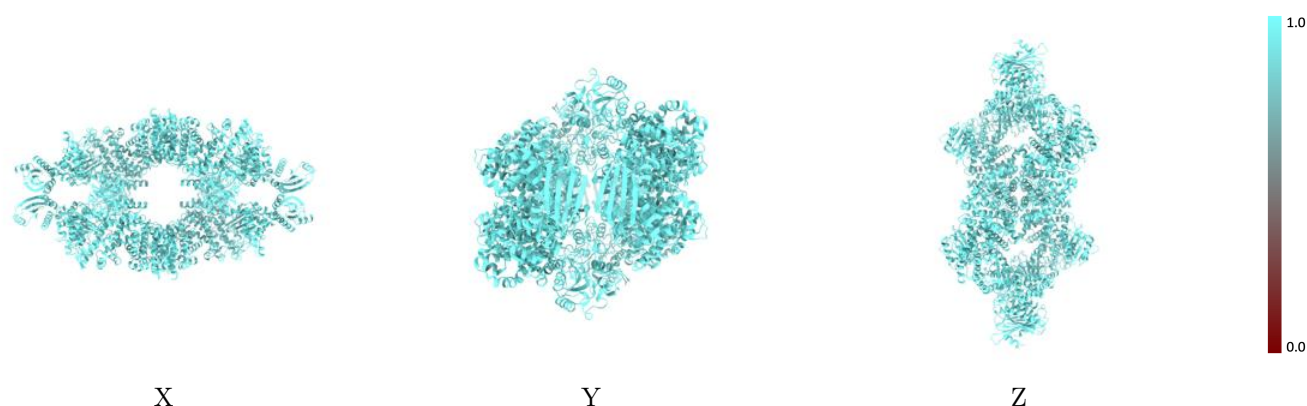
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



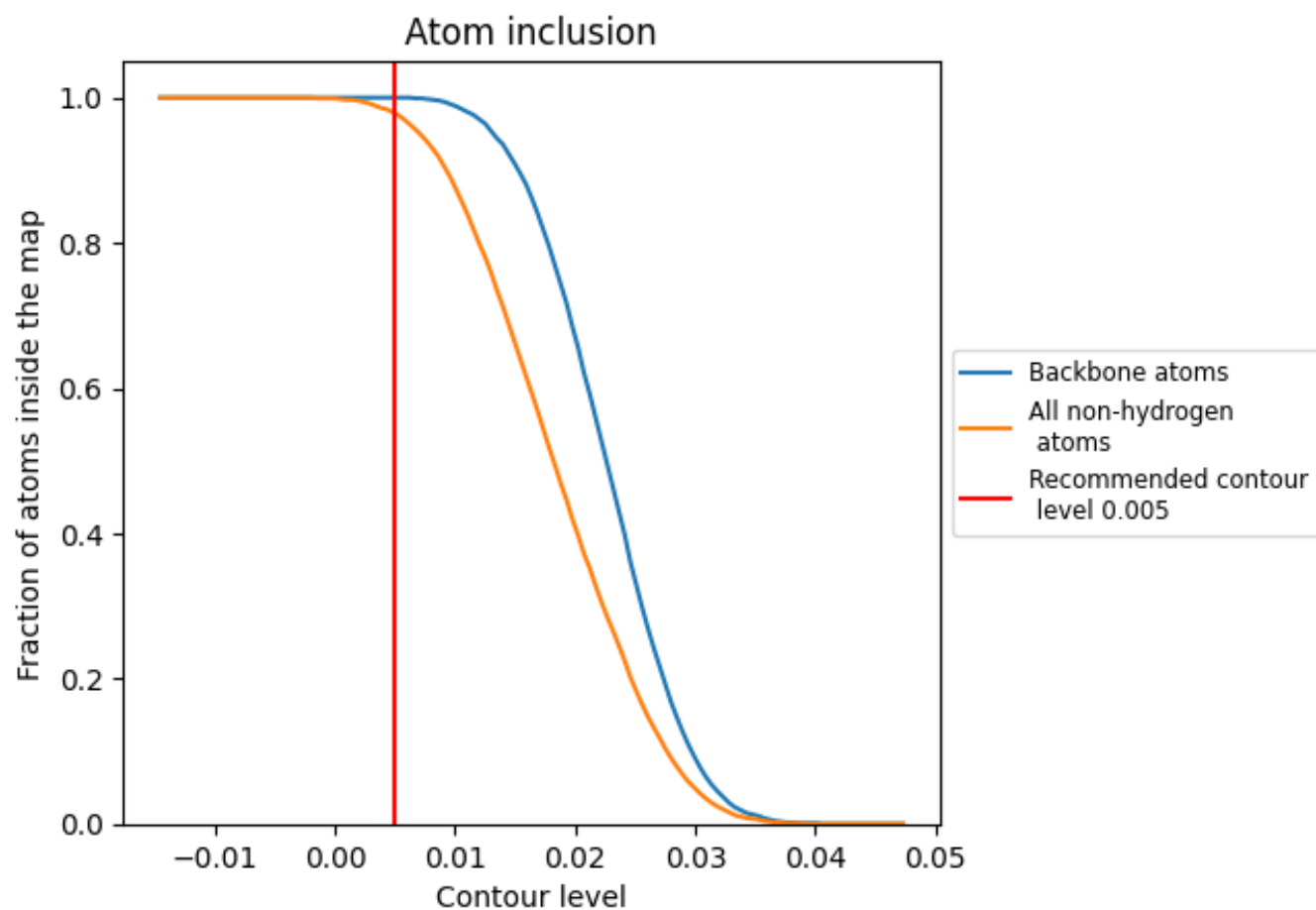
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9780	<div></div> 0.2920
A	<div></div> 0.9780	<div></div> 0.2920
B	<div></div> 0.9790	<div></div> 0.2920
C	<div></div> 0.9780	<div></div> 0.2930
D	<div></div> 0.9780	<div></div> 0.2930

