



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 05:42 AM UTC

PDB ID : 7B9K / pdb_00007b9k
EMDB ID : EMD-12104
Title : Cryo-EM structure of the dihydrolipoyl transacetylase cubic core of the E. coli pyruvate dehydrogenase complex including lipoyl domains
Authors : Skerlova, J.; Stenmark, P.
Deposited on : 2020-12-14
Resolution : 3.16 Å (reported)
Based on initial models : 4N72, 1QJO

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:

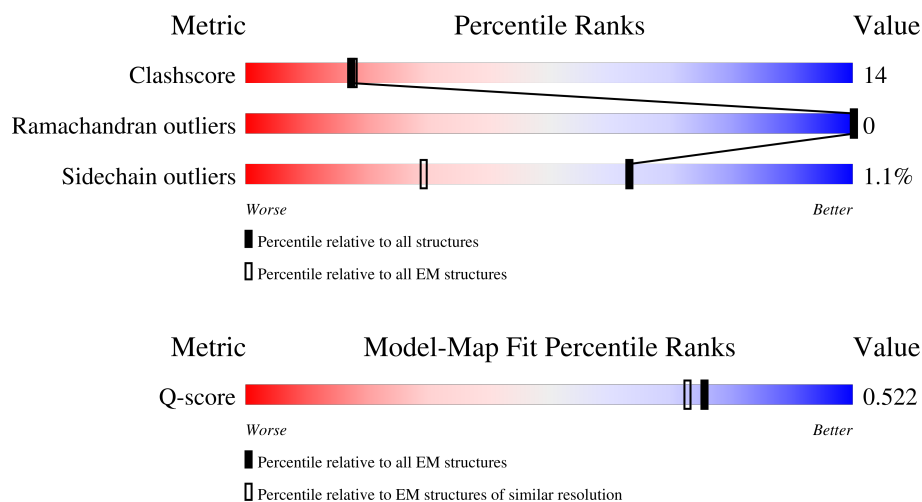
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.16 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	14474 (2.66 - 3.66)

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	630	8% 36% 14% 49%
1	B	630	7% 36% 14% 49%
1	C	630	8% 36% 14% 49%
1	D	630	8% 36% 15% 49%

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Mol	Chain	Length	Quality of chain
1	E	630	
1	F	630	
1	G	630	
1	H	630	
1	I	630	
1	J	630	
1	K	630	
1	L	630	
1	M	630	
1	N	630	
1	O	630	
1	P	630	
1	Q	630	
1	R	630	
1	S	630	
1	T	630	
1	U	630	
1	V	630	
1	W	630	
1	X	630	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 59136 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 Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	B	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	C	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	D	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	E	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	F	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	G	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	H	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	I	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	J	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	K	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	L	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	M	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	N	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	O	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		
1	P	320	Total	C	N	O	S	0	0
			2464	1572	416	461	15		

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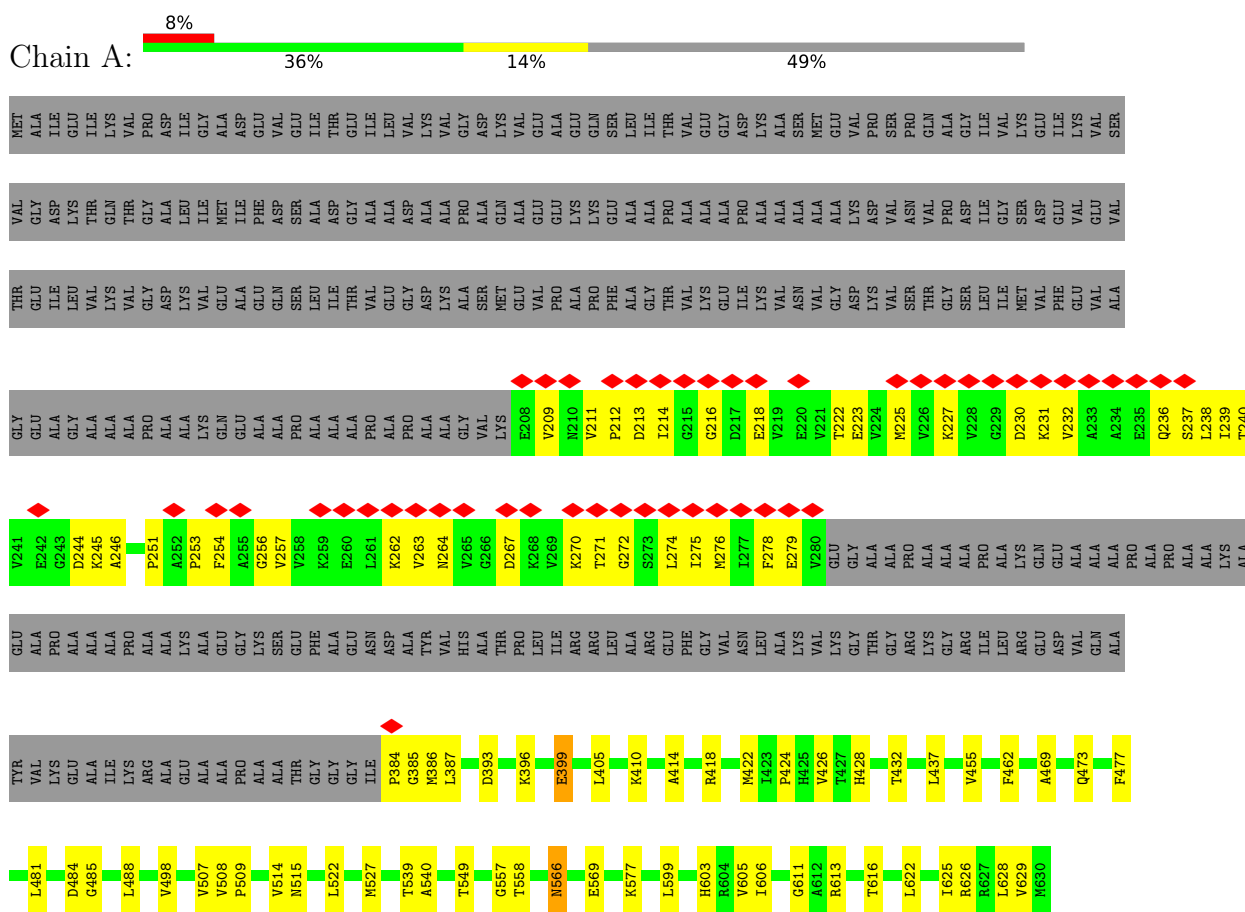
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	320	Total 2464	C 1572	N 416	O 461	S 15	0	0
1	R	320	Total 2464	C 1572	N 416	O 461	S 15	0	0
1	S	320	Total 2464	C 1572	N 416	O 461	S 15	0	0
1	T	320	Total 2464	C 1572	N 416	O 461	S 15	0	0
1	U	320	Total 2464	C 1572	N 416	O 461	S 15	0	0
1	V	320	Total 2464	C 1572	N 416	O 461	S 15	0	0
1	W	320	Total 2464	C 1572	N 416	O 461	S 15	0	0
1	X	320	Total 2464	C 1572	N 416	O 461	S 15	0	0

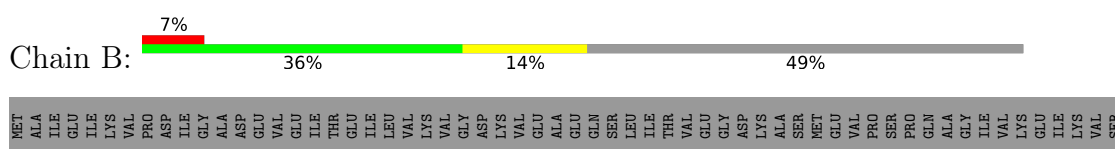
3 Residue-property plots

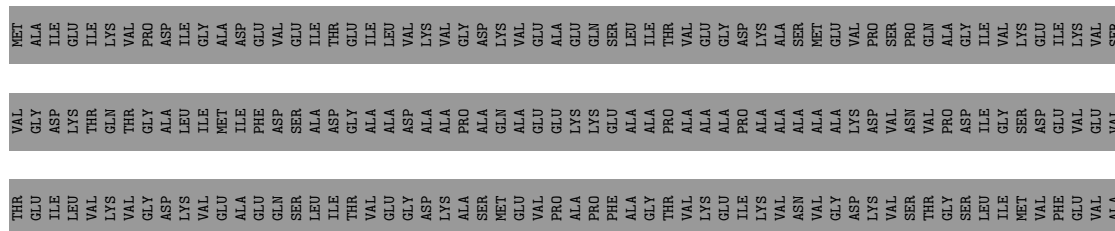
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

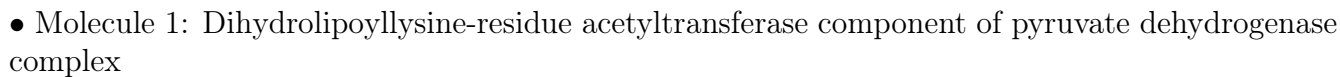
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

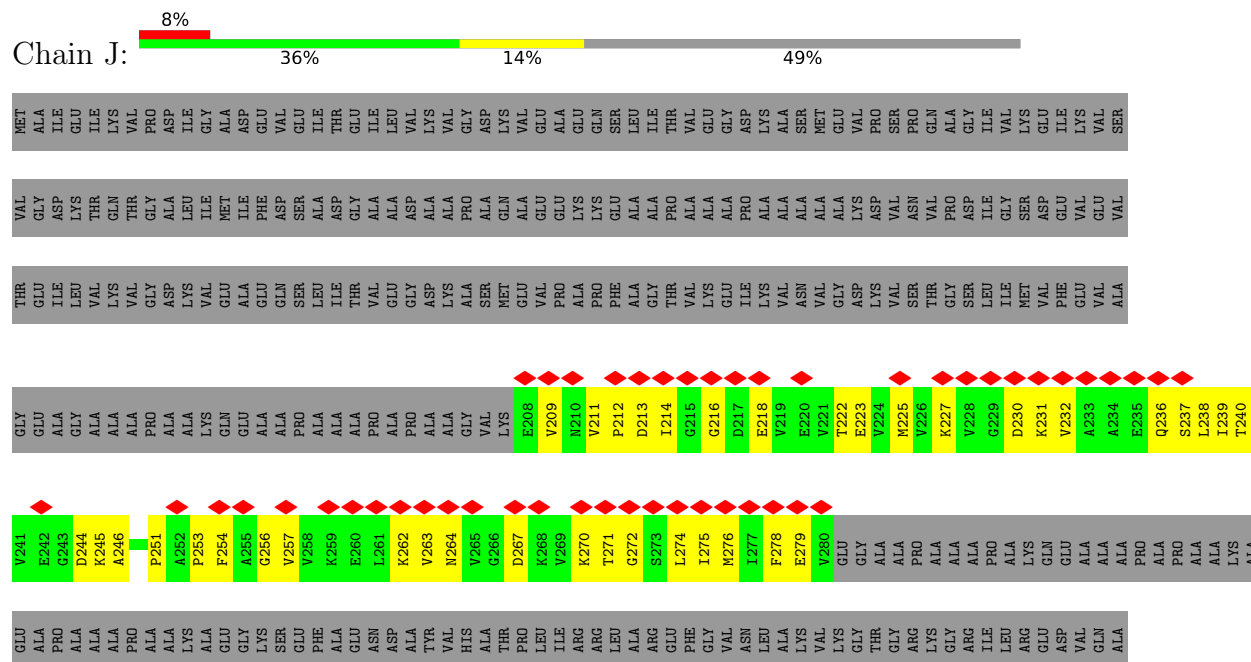
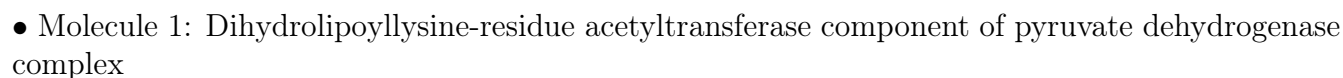


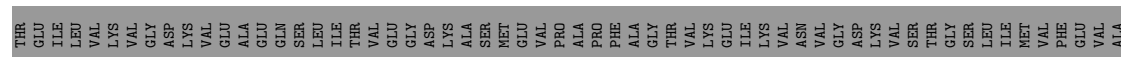
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

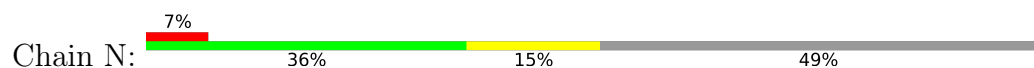


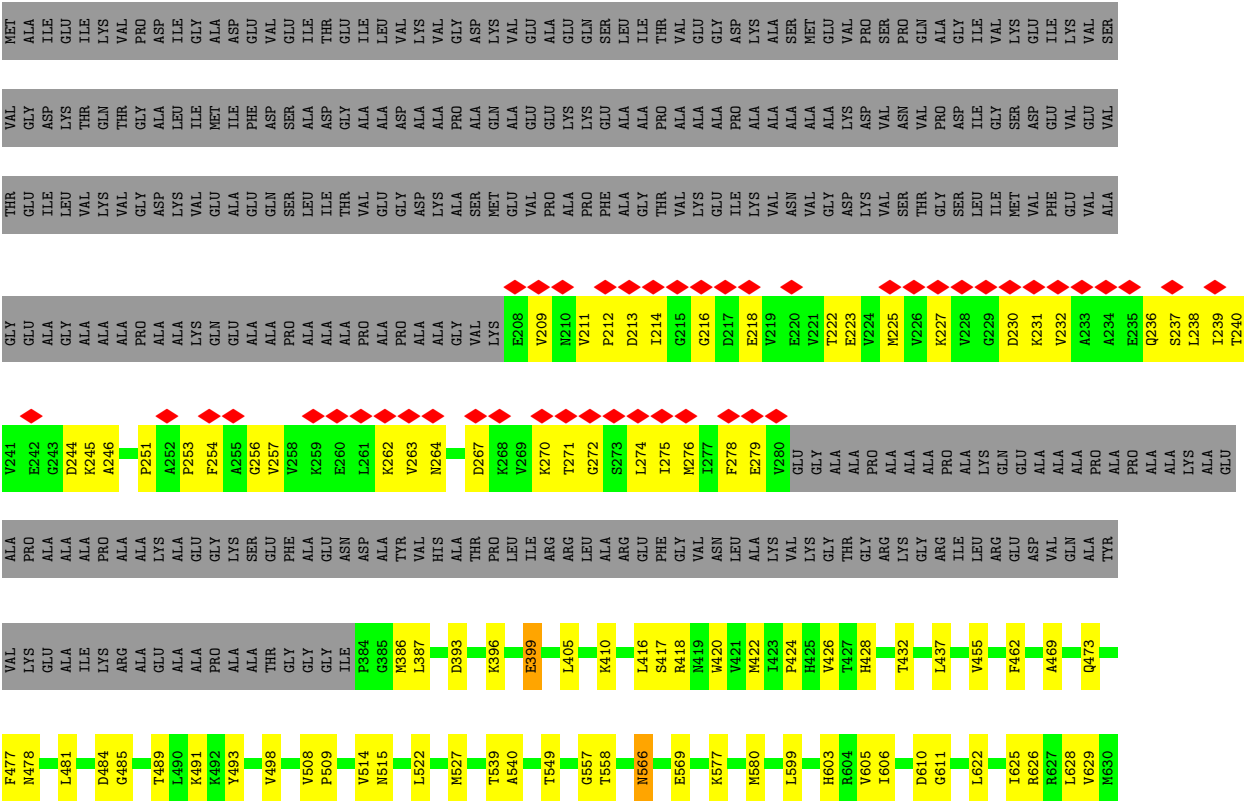




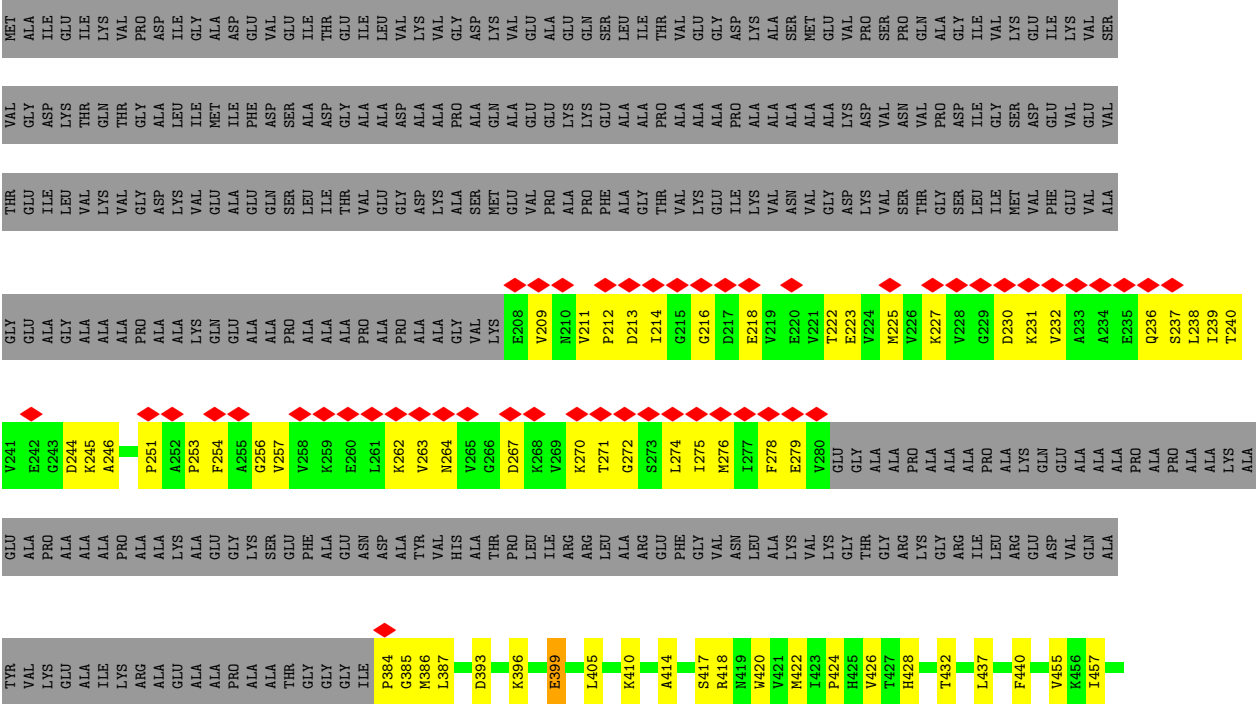
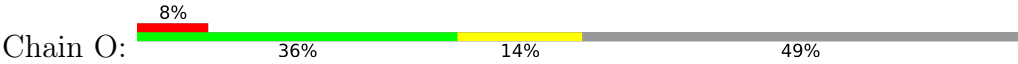




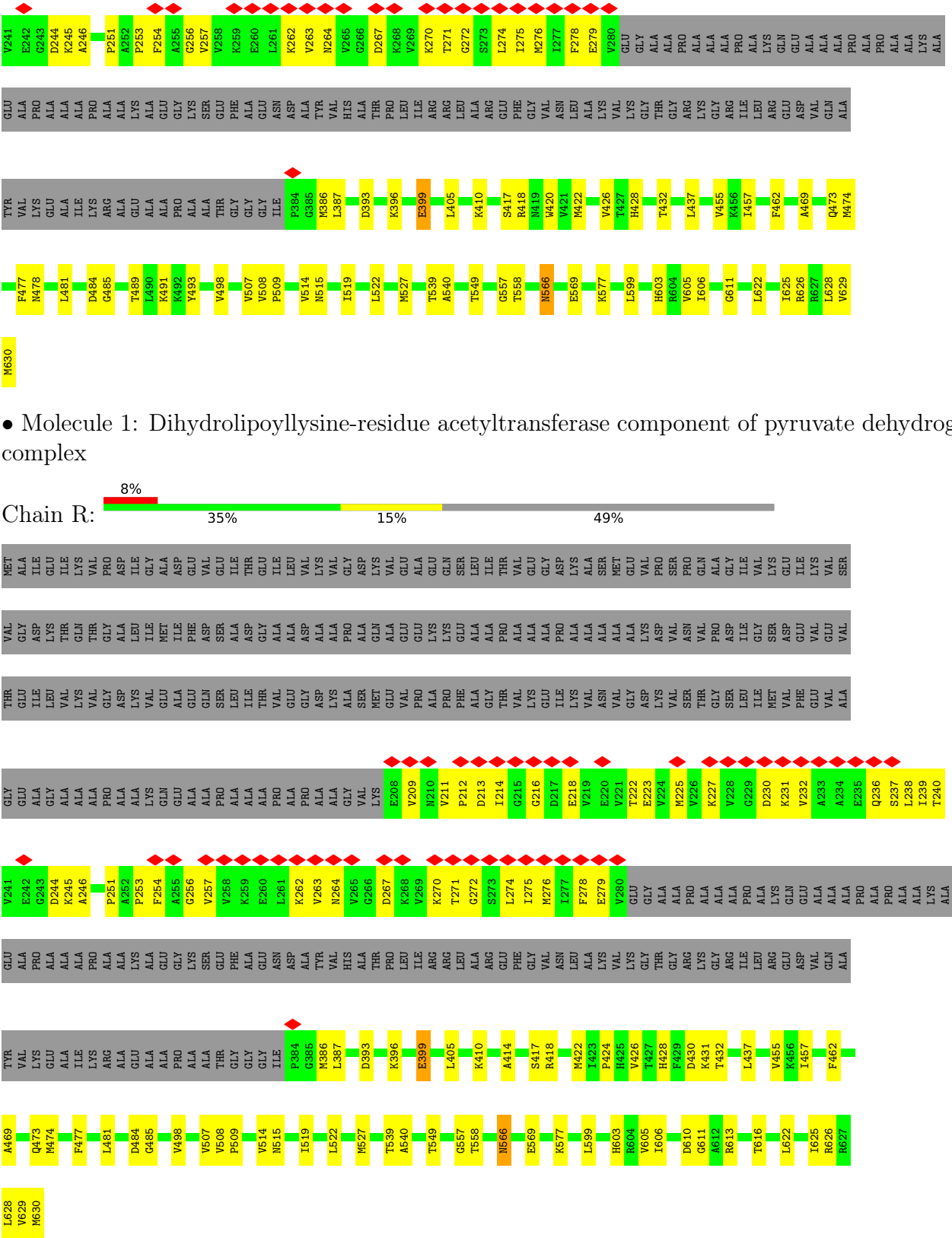




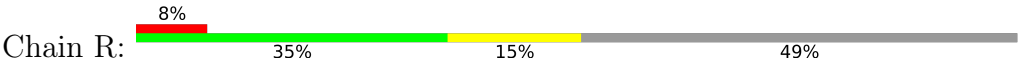
● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex



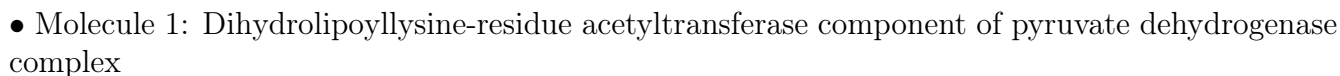


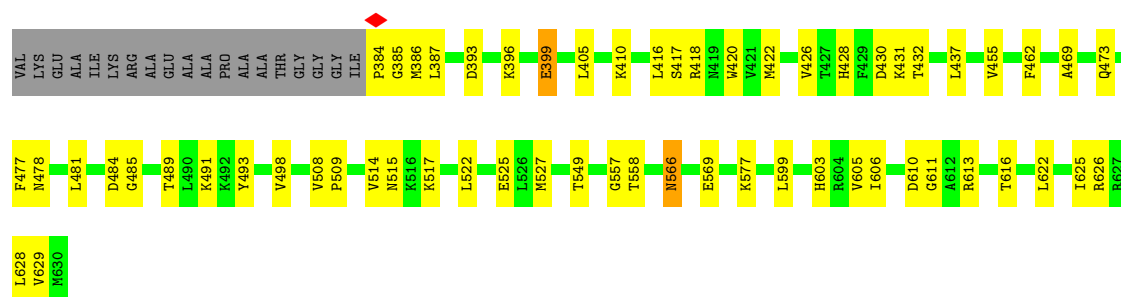


● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

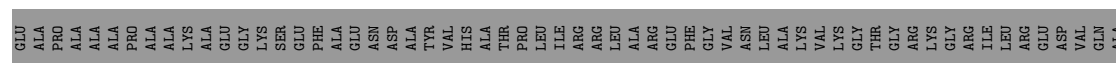
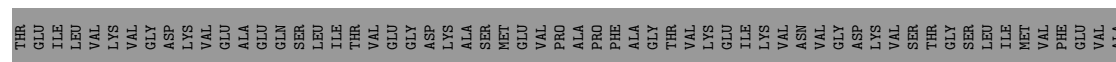
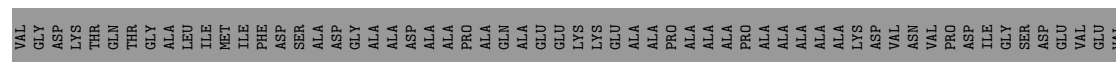
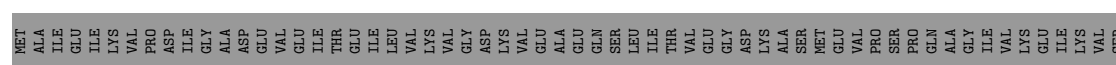
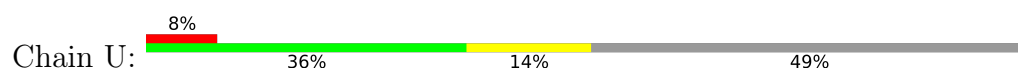


● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

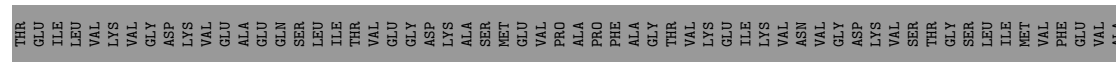
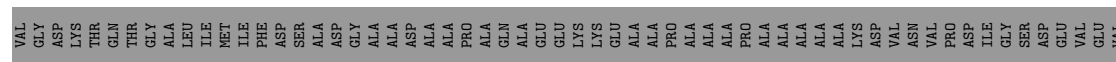
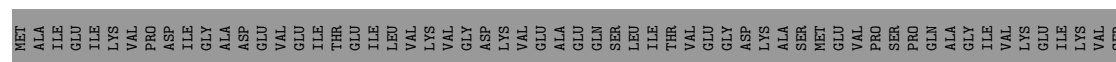
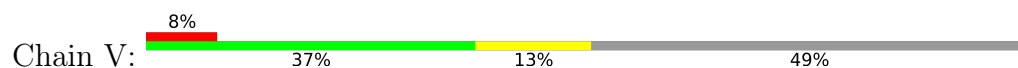




- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex



- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex



L628	F477	Tyr	GLU	V241	GLY	THR	VAL	MET
V629	L431	Val	ALA	G242	GLU	GLU	GLY	ALA
M630	L431	Lys	PRO	G243	ALA	ILE	ASP	GLU
		ALA	ALA	D244	ALA	VAL	THR	LYS
	D434	ILE	ALA	K245	ALA	LYS	GLN	LYS
	G485	Lys	PRO	A246	ALA	VAL	THR	VAL
	V498	Arg	ALA	P251	ALA	GLY	THR	GLY
	V507	GLU	LYS	K252	ALA	VAL	ILE	ALA
	V508	ALA	ALA	P253	ALA	LYS	MET	GLY
	P509	ALA	GLU	F254	ALA	VAL	ILE	ASP
		PRO	GLY	K255	GLU	ALA	ILE	ASP
	V514	ALA	LYS	G256	ALA	GLN	ILE	GLU
	M515	ALA	SER	V257	ALA	GLN	PHE	VAL
	K516	THR	GLU	V258	PRO	SER	ASP	GLU
	K517	GLY	PHE	K259	ALA	LEU	ILE	ILE
	G518	GLY	GLU	E260	ALA	ILE	ASP	THR
	I519	ILE	ASN	L261	PRO	VAL	GLY	ILE
		P384	ASP	K262	ALA	GLU	ALA	VAL
	L522	L387	ALA	V263	PRO	GLY	ASP	LEU
	E525	VAL	TYR	K264	ALA	ASP	ALA	LYS
	L526	D393	HIS	V265	ALA	LYS	ALA	VAL
	M527	ALA	ALA	G266	GLY	ALA	PRO	GLY
	T539	K396	THR	D267	LYS	MET	ALA	LYS
	A540	E399	PRO	K268	E208	GLU	ALA	VAL
	T549	L405	LEU	V269	V209	VAL	GLU	GLU
	G557	K410	ARG	K270	N210	PRO	LYS	ALA
	T558	A414	LEU	T271	P212	PHE	GLU	LEU
	M566	R418	ARG	G272	D213	ALA	ALA	ILE
	E569	R418	GLU	S273	T214	THR	PRO	THR
	K577	M422	PHE	L274	G215	VAL	ALA	VAL
	L589	I433	VAL	T275	G216	LYS	ALA	GLY
	M603	P424	ASN	M276	D217	GLU	ALA	ASP
	V605	V426	LEU	T277	E218	ILE	PRO	LYS
	I606	H428	LYS	F278	V219	VAL	ALA	LYS
		T432	VAL	E279	A220	ASN	ALA	SER
	D610	L437	LYS	V280	V221	VAL	ALA	MET
	G611	V455	GLY	GLU	T222	GLY	ALA	GLU
	A612	K456	THR	GLY	E223	ASP	ALA	VAL
	R613	I457	ARG	ALA	V224	LYS	LYS	PRO
	T616	F462	ILE	ALA	N225	VAL	VAL	PRO
	L622	A469	LEU	ALA	V226	SER	ASN	PRO
	I625		ARG	LYS	K227	THR	VAL	GLN
	R626		GLU	ALA	V228	GLY	PRO	ALA
	R627	Q473	ASP	PRO	G229	SER	ASP	ALA
		M474	VAL	ALA	D230	LEU	ILE	VAL
			GLN	ALA	K231	ILE	GLY	LYS
			ALA	ALA	V232	MET	SER	GLU
			ALA	ALA	A233	PHE	ASP	ILE
			PRO	ALA	K234	VAL	GLU	LYS
			ALA	ALA	E235	GLU	VAL	VAL
			ALA	ALA	Q236	VAL	GLU	SER
			PRO	ALA	S237	ALA	VAL	VAL
			PRO	ALA	L238	LYS	GLU	VAL
			LYS	ALA	T240		VAL	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	29434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30, 28.11, 28.11	Depositor
Minimum defocus (nm)	Not provided, Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided, Not provided	Depositor
Magnification	Not provided, Not provided, Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k), GATAN K2 QUANTUM (4k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.683	Depositor
Minimum map value	-1.210	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LA2

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	0/2482	0.42	0/3349
1	B	0.25	0/2482	0.42	0/3349
1	C	0.25	0/2482	0.42	0/3349
1	D	0.25	0/2482	0.42	0/3349
1	E	0.25	0/2482	0.42	0/3349
1	F	0.25	0/2482	0.42	0/3349
1	G	0.25	0/2482	0.42	0/3349
1	H	0.25	0/2482	0.42	0/3349
1	I	0.25	0/2482	0.42	0/3349
1	J	0.25	0/2482	0.42	0/3349
1	K	0.25	0/2482	0.42	0/3349
1	L	0.25	0/2482	0.42	0/3349
1	M	0.25	0/2482	0.42	0/3349
1	N	0.25	0/2482	0.42	0/3349
1	O	0.25	0/2482	0.42	0/3349
1	P	0.25	0/2482	0.42	0/3349
1	Q	0.25	0/2482	0.42	0/3349
1	R	0.25	0/2482	0.42	0/3349
1	S	0.25	0/2482	0.42	0/3349
1	T	0.25	0/2482	0.42	0/3349
1	U	0.25	0/2482	0.42	0/3349
1	V	0.25	0/2482	0.42	0/3349
1	W	0.25	0/2482	0.42	0/3349
1	X	0.25	0/2482	0.42	0/3349
All	All	0.25	0/59568	0.42	0/80376

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 ⓘ

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	2464	0	2550	75	0
1	B	2464	0	2550	74	0
1	C	2464	0	2550	78	0
1	D	2464	0	2550	82	0
1	E	2464	0	2550	79	0
1	F	2464	0	2550	72	0
1	G	2464	0	2550	78	0
1	H	2464	0	2550	82	0
1	I	2464	0	2550	76	0
1	J	2464	0	2550	76	0
1	K	2464	0	2550	77	0
1	L	2464	0	2550	82	0
1	M	2464	0	2550	79	0
1	N	2464	0	2550	79	0
1	O	2464	0	2550	85	0
1	P	2464	0	2550	83	0
1	Q	2464	0	2550	79	0
1	R	2464	0	2550	82	0
1	S	2464	0	2550	77	0
1	T	2464	0	2550	81	0
1	U	2464	0	2550	82	0
1	V	2464	0	2550	74	0
1	W	2464	0	2550	76	0
1	X	2464	0	2550	81	0
All	All	59136	0	61200	1635	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 14.

The worst 5 of 1635 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:E:426:VAL:HG21	1:E:603:HIS:HD2	1.28	0.99
1:F:426:VAL:HG21	1:F:603:HIS:HD2	1.28	0.99
1:S:426:VAL:HG21	1:S:603:HIS:HD2	1.28	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:426:VAL:HG21	1:U:603:HIS:HD2	1.28	0.99
1:O:426:VAL:HG21	1:O:603:HIS:HD2	1.28	0.98

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	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	B	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	C	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	D	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	E	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	F	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	G	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	H	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	I	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	J	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	K	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	L	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	M	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	N	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	O	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	P	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	Q	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	R	315/630 (50%)	300 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	T	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	U	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	V	315/630 (50%)	299 (95%)	16 (5%)	0	100	100
1	W	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
1	X	315/630 (50%)	300 (95%)	15 (5%)	0	100	100
All	All	7560/15120 (50%)	7188 (95%)	372 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	B	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	C	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	D	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	E	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	F	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	G	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	H	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	I	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	J	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	K	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	L	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	M	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	N	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	O	271/482 (56%)	268 (99%)	3 (1%)	65	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	Q	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	R	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	S	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	T	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	U	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	V	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	W	271/482 (56%)	268 (99%)	3 (1%)	65	75
1	X	271/482 (56%)	268 (99%)	3 (1%)	65	75
All	All	6504/11568 (56%)	6432 (99%)	72 (1%)	63	75

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	213	ASP
1	X	566	ASN
1	T	566	ASN
1	V	566	ASN
1	I	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	236	GLN
1	R	236	GLN
1	Q	236	GLN
1	S	236	GLN
1	G	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

24 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LA2	V	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	K	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	I	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	W	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	G	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	S	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	F	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	M	245	1	17,19,20	0.42	0	12,21,23	0.45	0
1	LA2	R	245	1	17,19,20	0.42	0	12,21,23	0.44	0
1	LA2	B	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	L	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	A	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	P	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	H	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	X	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	D	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	J	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	U	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	O	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	Q	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	T	245	1	17,19,20	0.41	0	12,21,23	0.45	0
1	LA2	N	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	E	245	1	17,19,20	0.41	0	12,21,23	0.44	0
1	LA2	C	245	1	17,19,20	0.41	0	12,21,23	0.44	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
1	LA2	V	245	1	-	6/18/20/22	-
1	LA2	K	245	1	-	6/18/20/22	-
1	LA2	I	245	1	-	6/18/20/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LA2	W	245	1	-	6/18/20/22	-
1	LA2	G	245	1	-	6/18/20/22	-
1	LA2	S	245	1	-	6/18/20/22	-
1	LA2	F	245	1	-	6/18/20/22	-
1	LA2	M	245	1	-	6/18/20/22	-
1	LA2	R	245	1	-	6/18/20/22	-
1	LA2	B	245	1	-	6/18/20/22	-
1	LA2	L	245	1	-	6/18/20/22	-
1	LA2	A	245	1	-	6/18/20/22	-
1	LA2	P	245	1	-	6/18/20/22	-
1	LA2	H	245	1	-	6/18/20/22	-
1	LA2	X	245	1	-	6/18/20/22	-
1	LA2	D	245	1	-	6/18/20/22	-
1	LA2	J	245	1	-	6/18/20/22	-
1	LA2	U	245	1	-	6/18/20/22	-
1	LA2	O	245	1	-	6/18/20/22	-
1	LA2	Q	245	1	-	6/18/20/22	-
1	LA2	T	245	1	-	6/18/20/22	-
1	LA2	N	245	1	-	6/18/20/22	-
1	LA2	E	245	1	-	6/18/20/22	-
1	LA2	C	245	1	-	6/18/20/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 144 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	245	LA2	O1-C1-NZ-CE
1	A	245	LA2	C2-C1-NZ-CE
1	A	245	LA2	C6-C7-C8-S8
1	B	245	LA2	O1-C1-NZ-CE
1	B	245	LA2	C2-C1-NZ-CE

There are no ring outliers.

24 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	V	245	LA2	3	0
1	K	245	LA2	4	0
1	I	245	LA2	4	0
1	W	245	LA2	5	0
1	G	245	LA2	4	0
1	S	245	LA2	3	0
1	F	245	LA2	4	0
1	M	245	LA2	3	0
1	R	245	LA2	5	0
1	B	245	LA2	5	0
1	L	245	LA2	3	0
1	A	245	LA2	3	0
1	P	245	LA2	2	0
1	H	245	LA2	5	0
1	X	245	LA2	4	0
1	D	245	LA2	4	0
1	J	245	LA2	3	0
1	U	245	LA2	3	0
1	O	245	LA2	5	0
1	Q	245	LA2	5	0
1	T	245	LA2	4	0
1	N	245	LA2	4	0
1	E	245	LA2	2	0
1	C	245	LA2	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

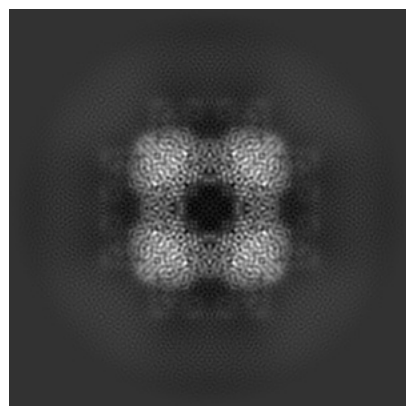
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12104. These allow visual inspection of the internal detail of the map and identification of artifacts.

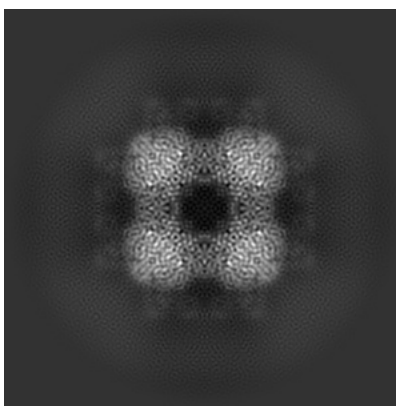
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

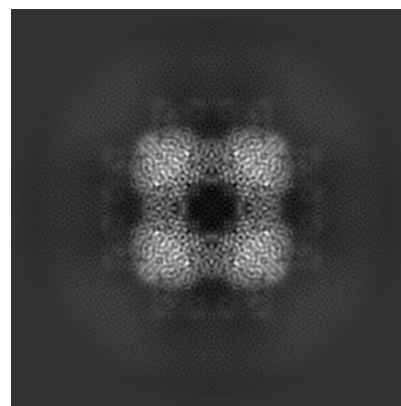
6.1.1 Primary map



X

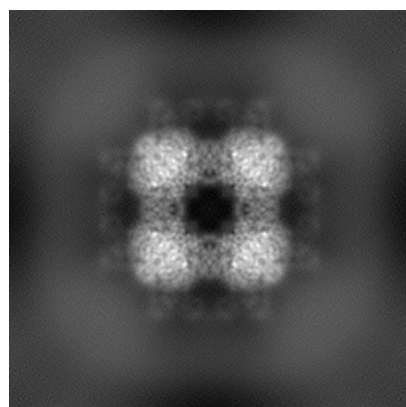


Y

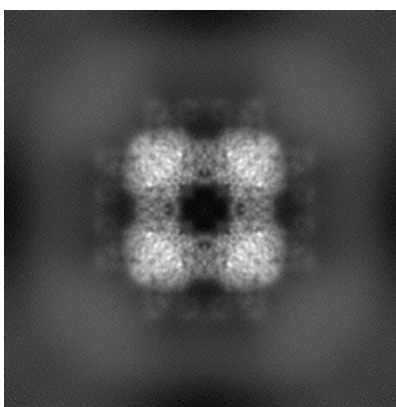


Z

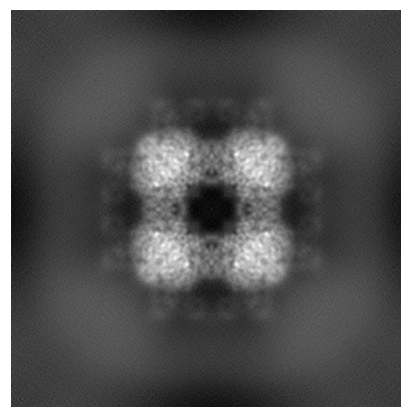
6.1.2 Raw map



X



Y

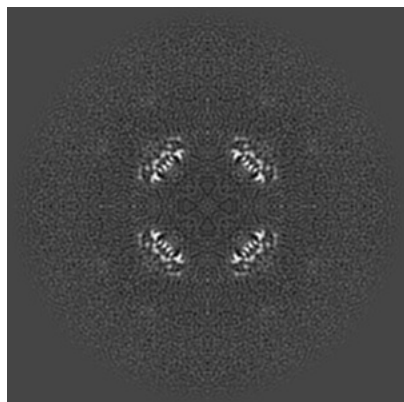


Z

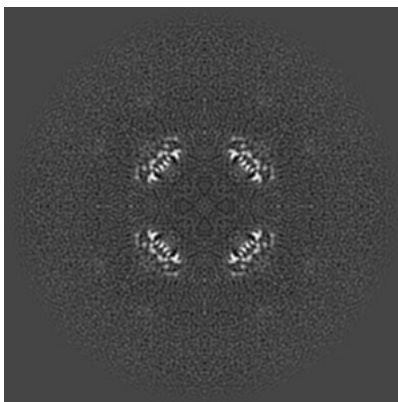
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

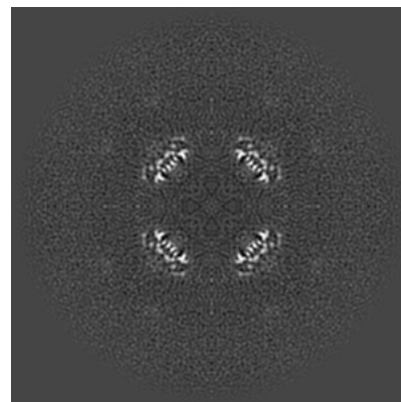
6.2.1 Primary map



X Index: 150

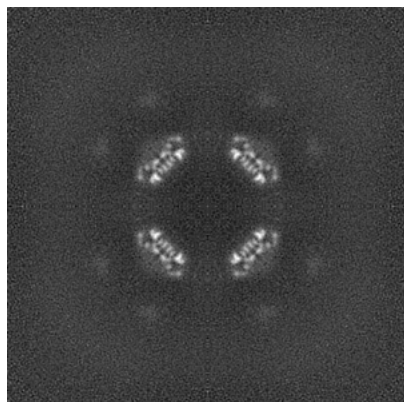


Y Index: 150

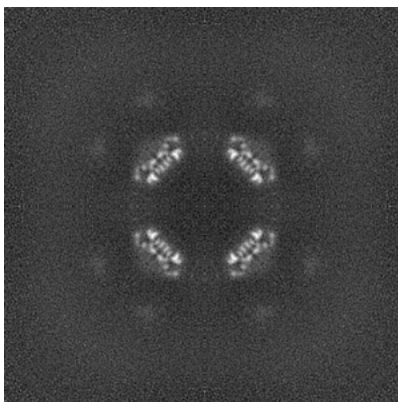


Z Index: 150

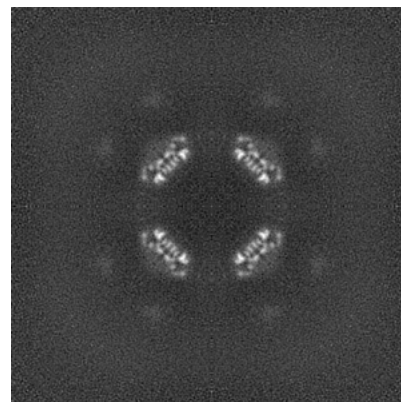
6.2.2 Raw map



X Index: 150



Y Index: 150

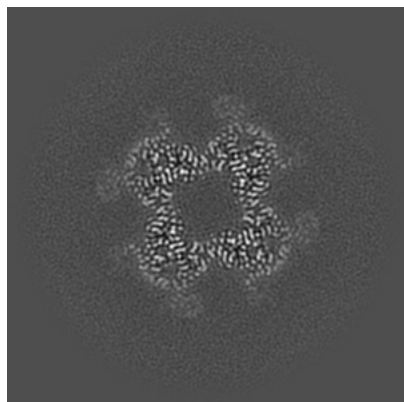


Z Index: 150

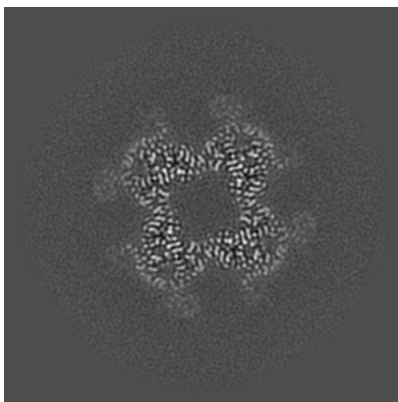
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

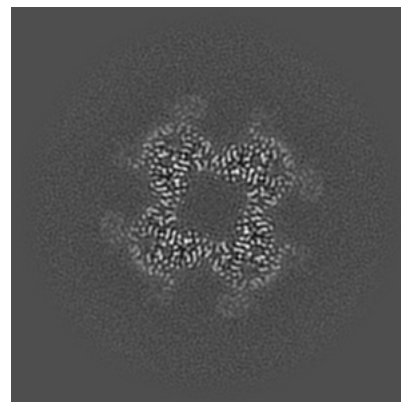
6.3.1 Primary map



X Index: 181

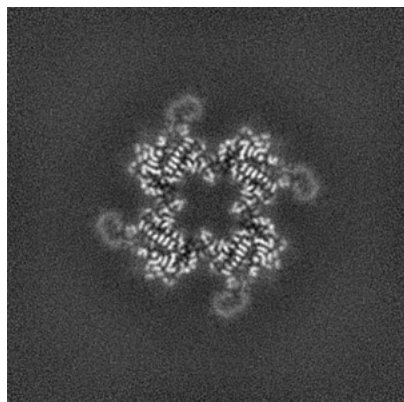


Y Index: 181

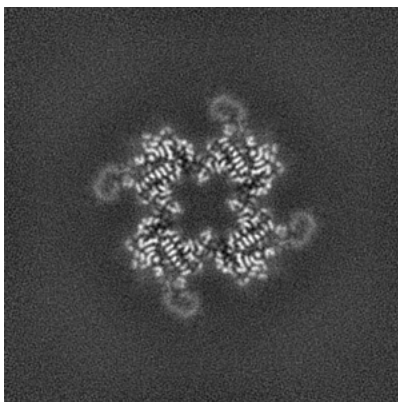


Z Index: 119

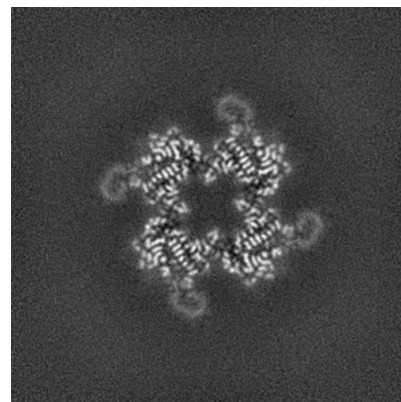
6.3.2 Raw map



X Index: 114



Y Index: 186

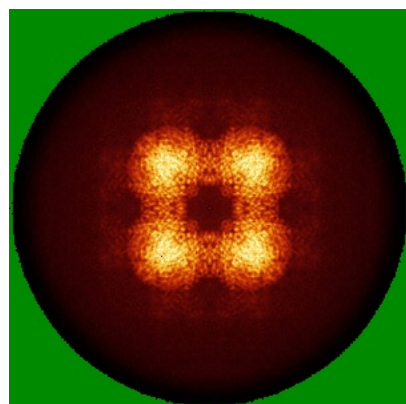


Z Index: 186

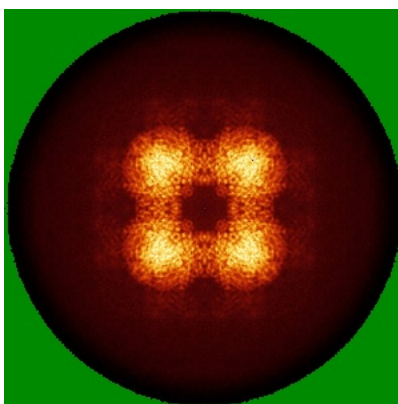
The images above show the largest variance slices of the map in three orthogonal directions.

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

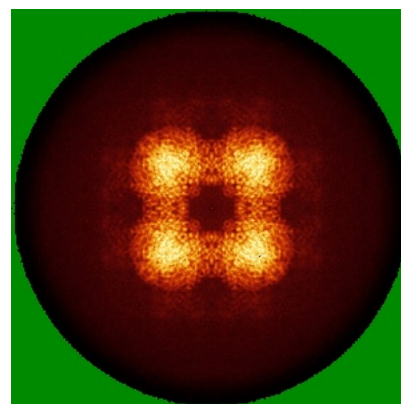
6.4.1 Primary map



X

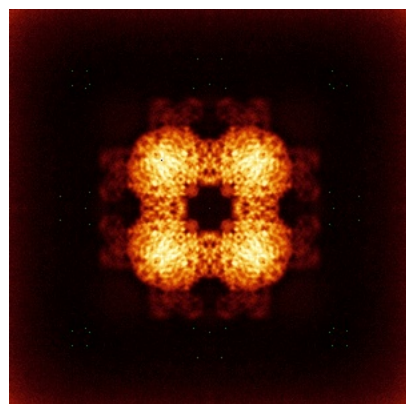


Y

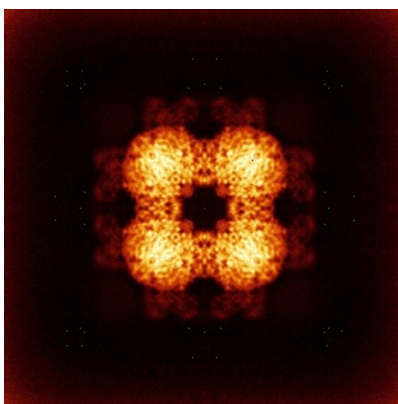


Z

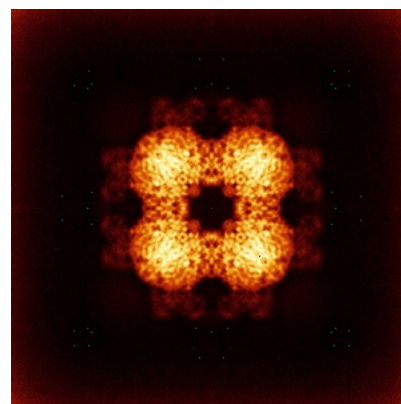
6.4.2 Raw map



X



Y

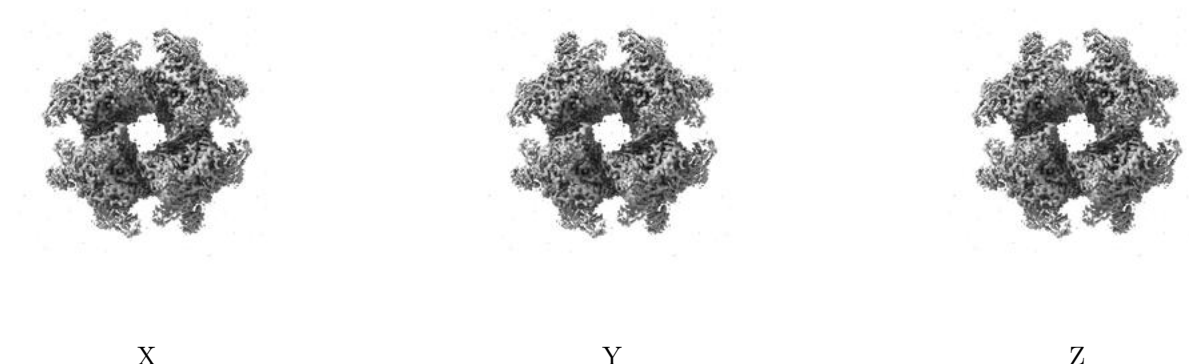


Z

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.

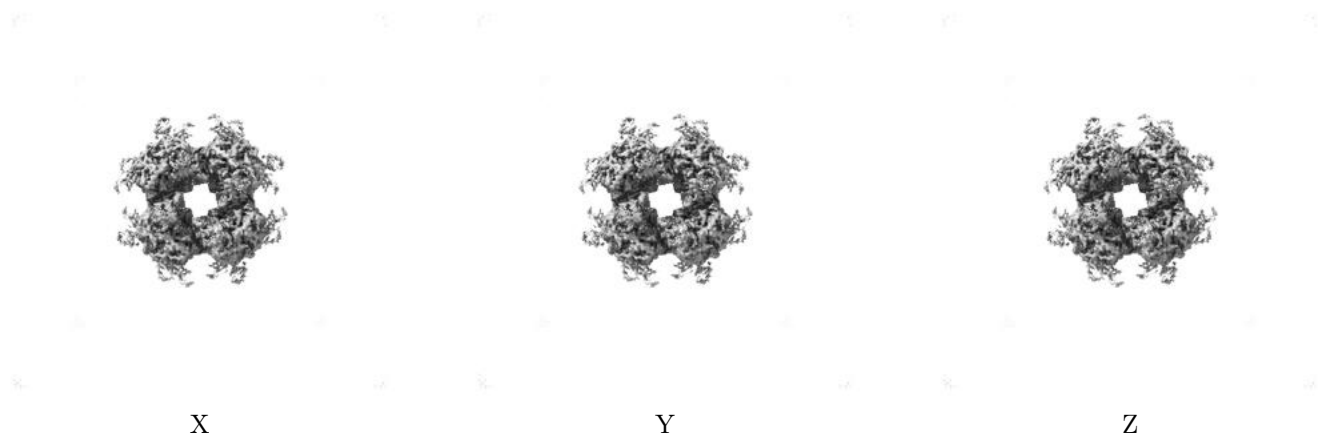
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

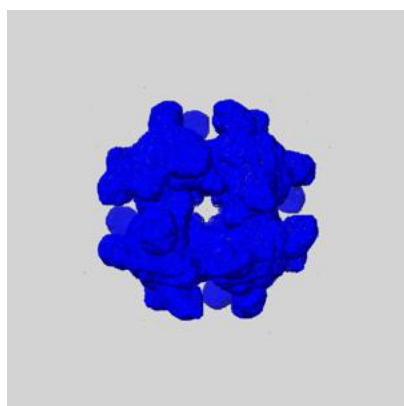
6.6 Mask visualisation [i](#)

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

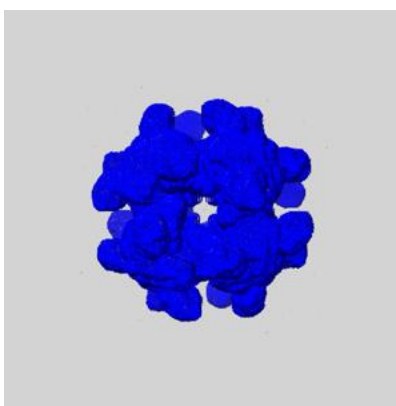
A mask typically either:

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

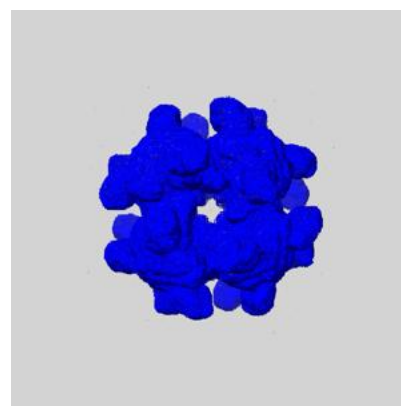
6.6.1 emd_12104_msk_1.map [i](#)



X



Y

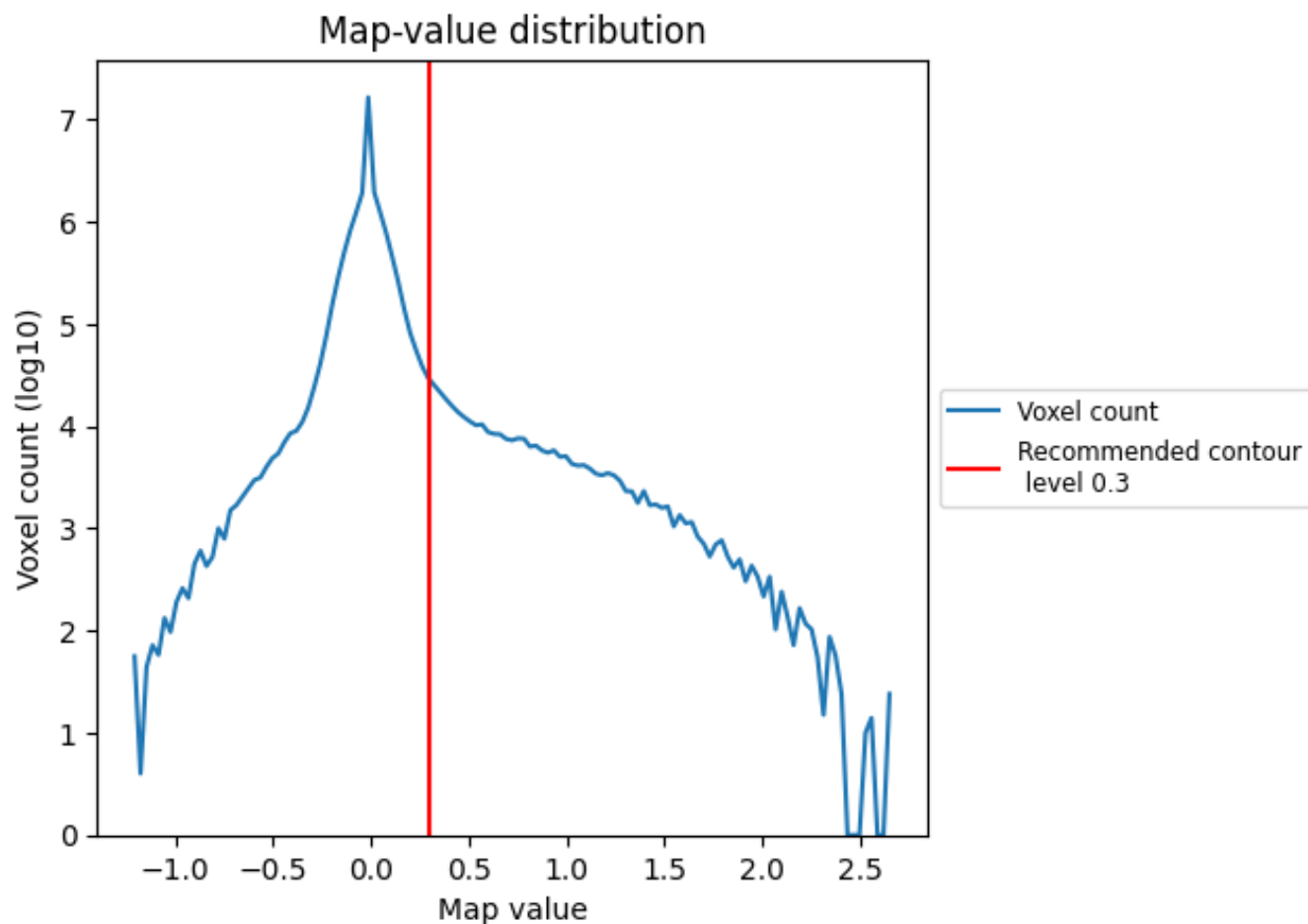


Z

7 Map analysis [i](#)

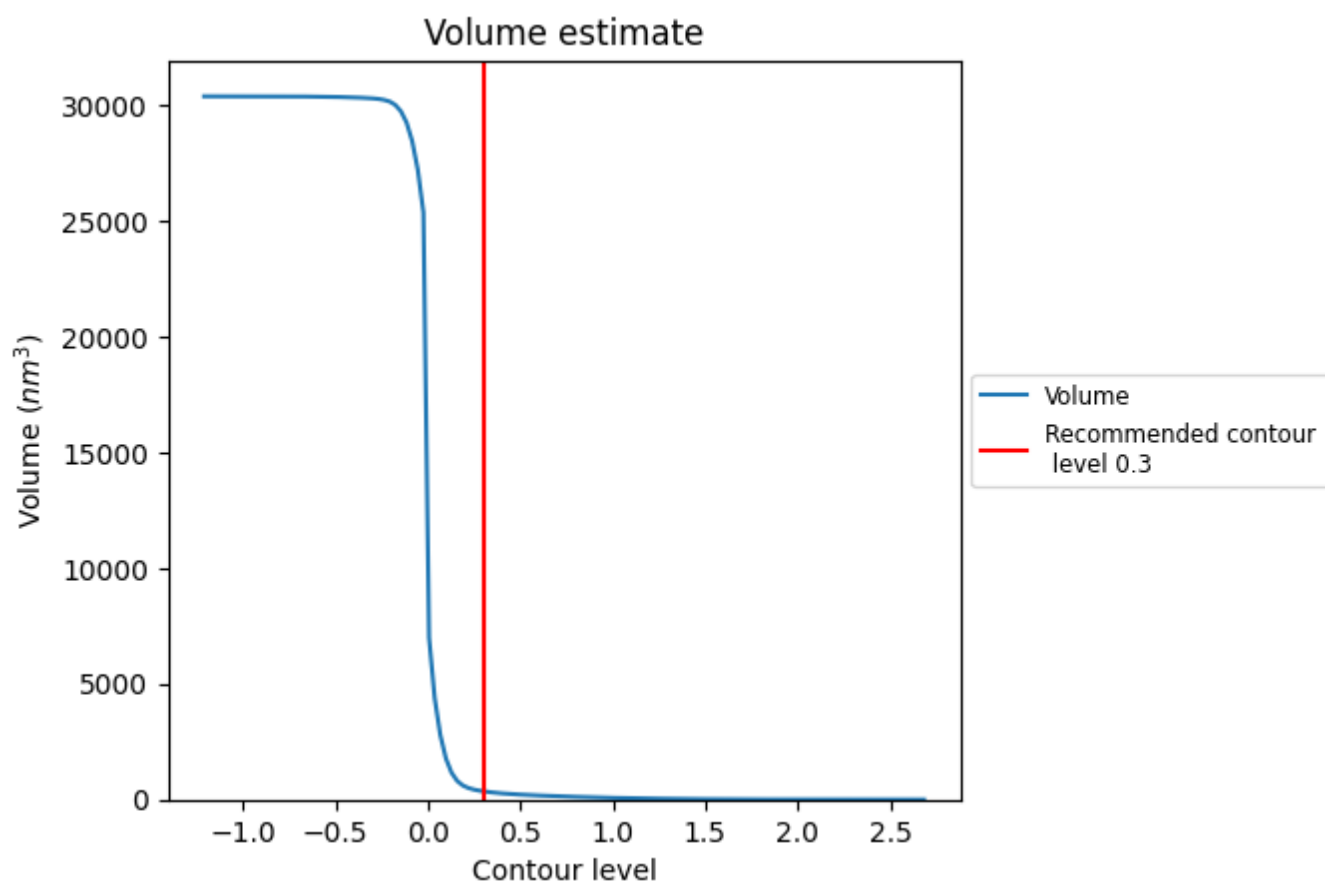
This section contains the results of statistical analysis of the map.

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.

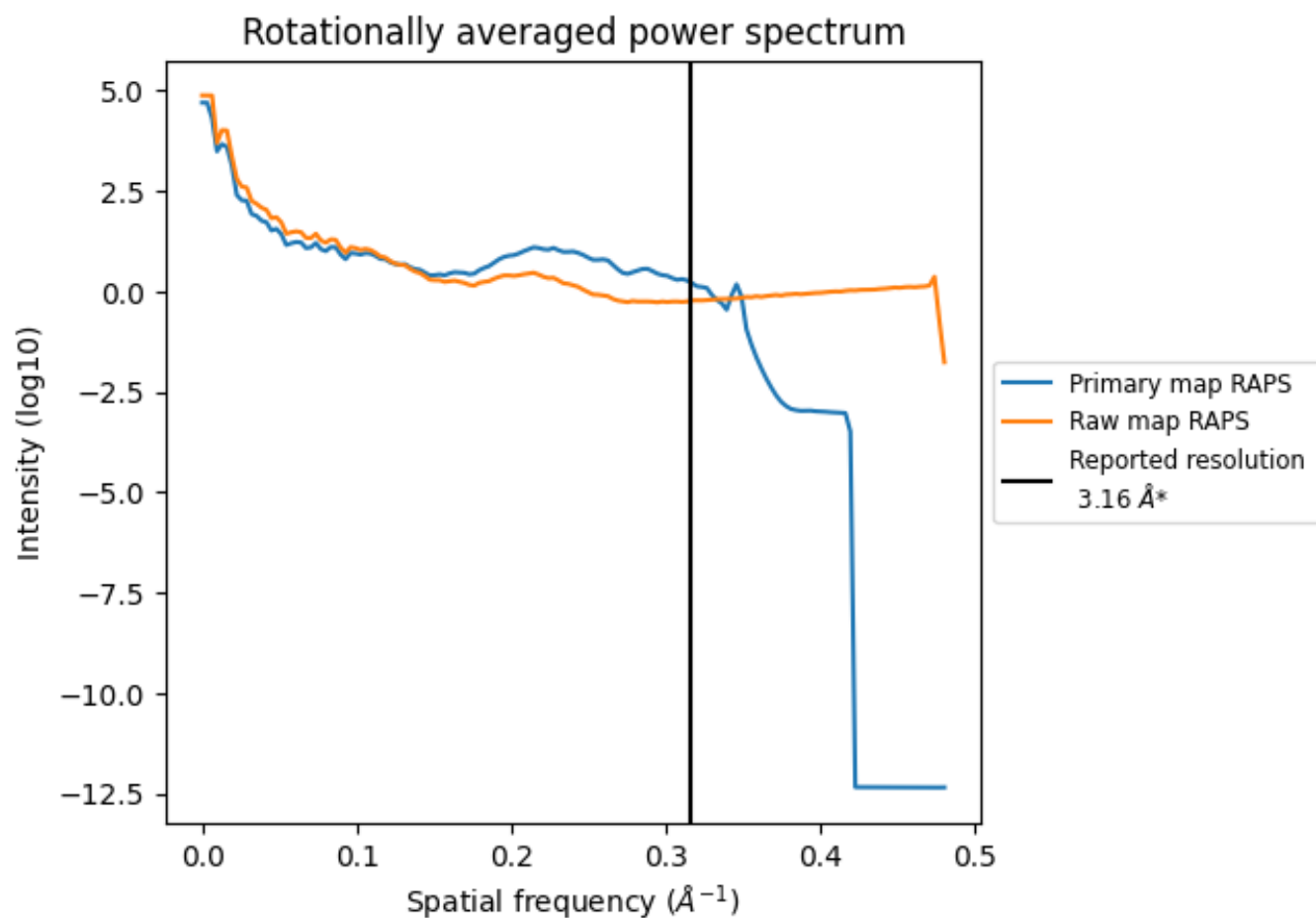
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 357 nm³; this corresponds to an approximate mass of 323 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 ⓘ

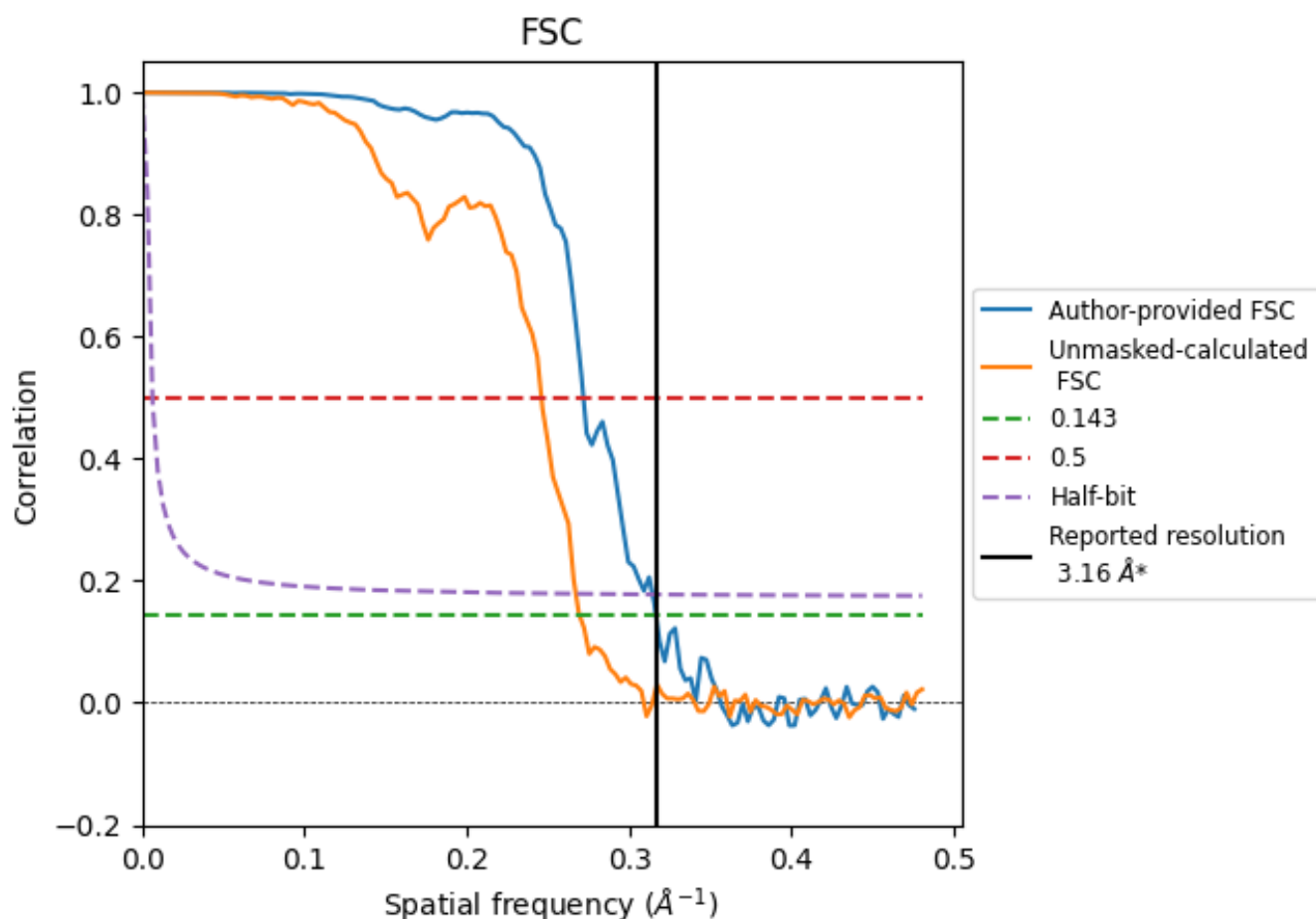


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8.2 Resolution estimates [i](#)

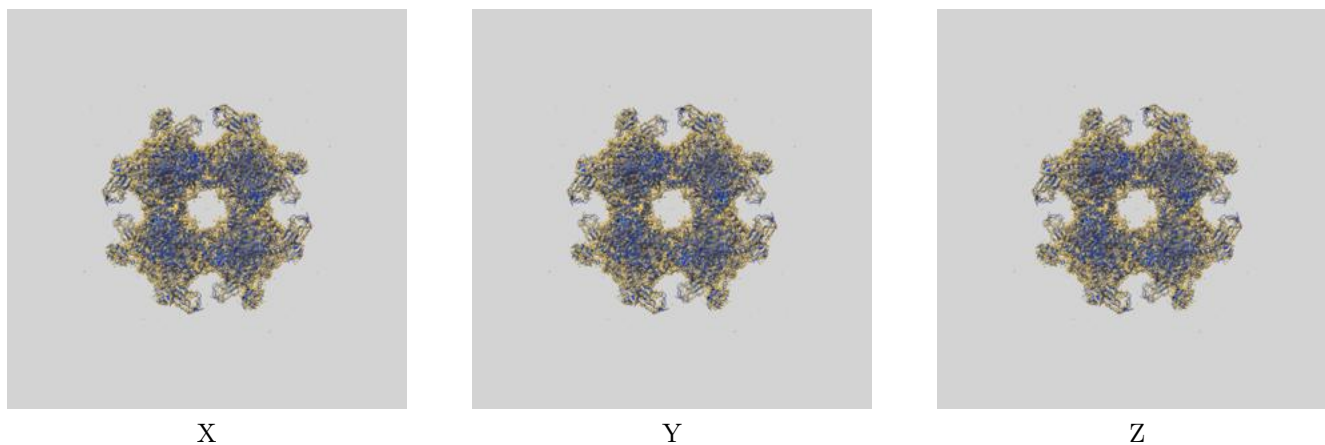
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.68	3.18
Unmasked-calculated*	3.71	4.06	3.74

*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 3.71 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

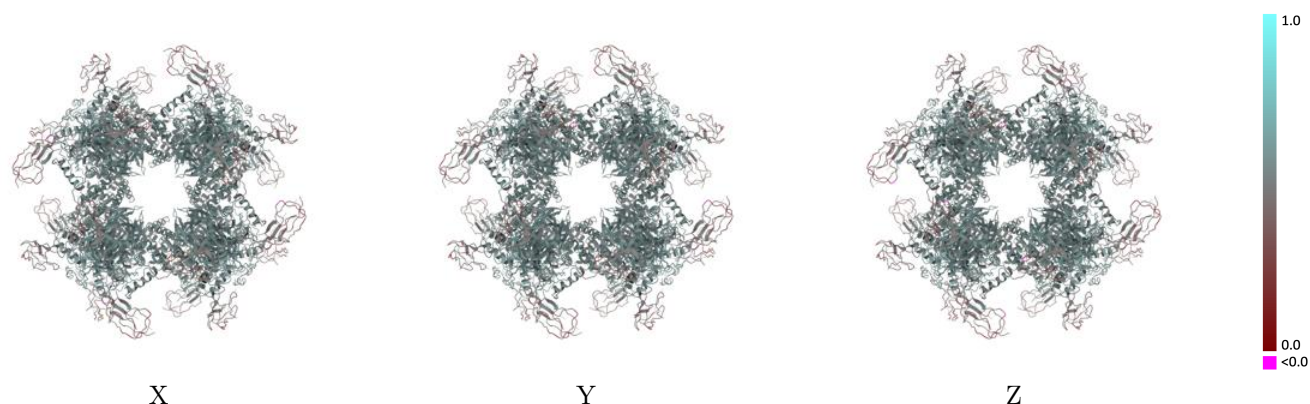
This section contains information regarding the fit between EMDB map EMD-12104 and PDB model 7B9K. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



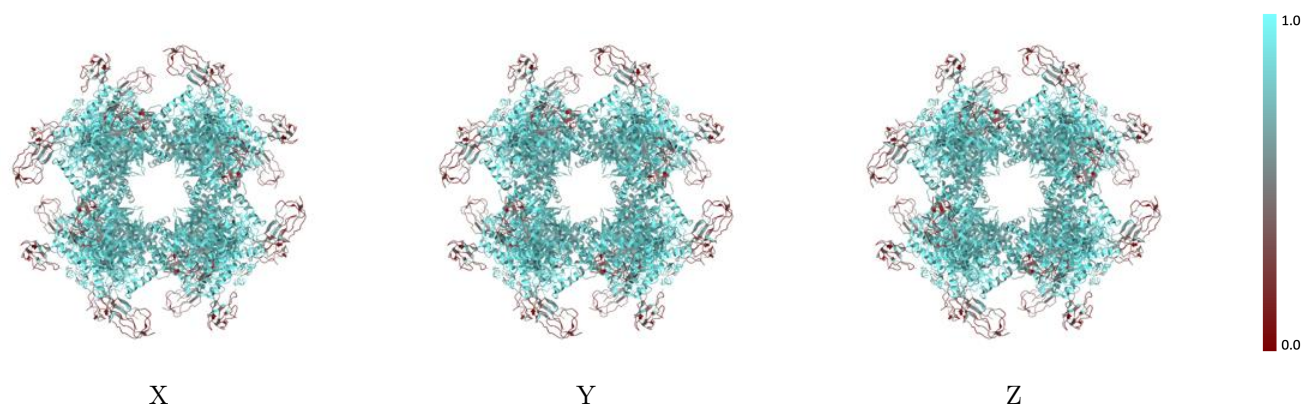
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



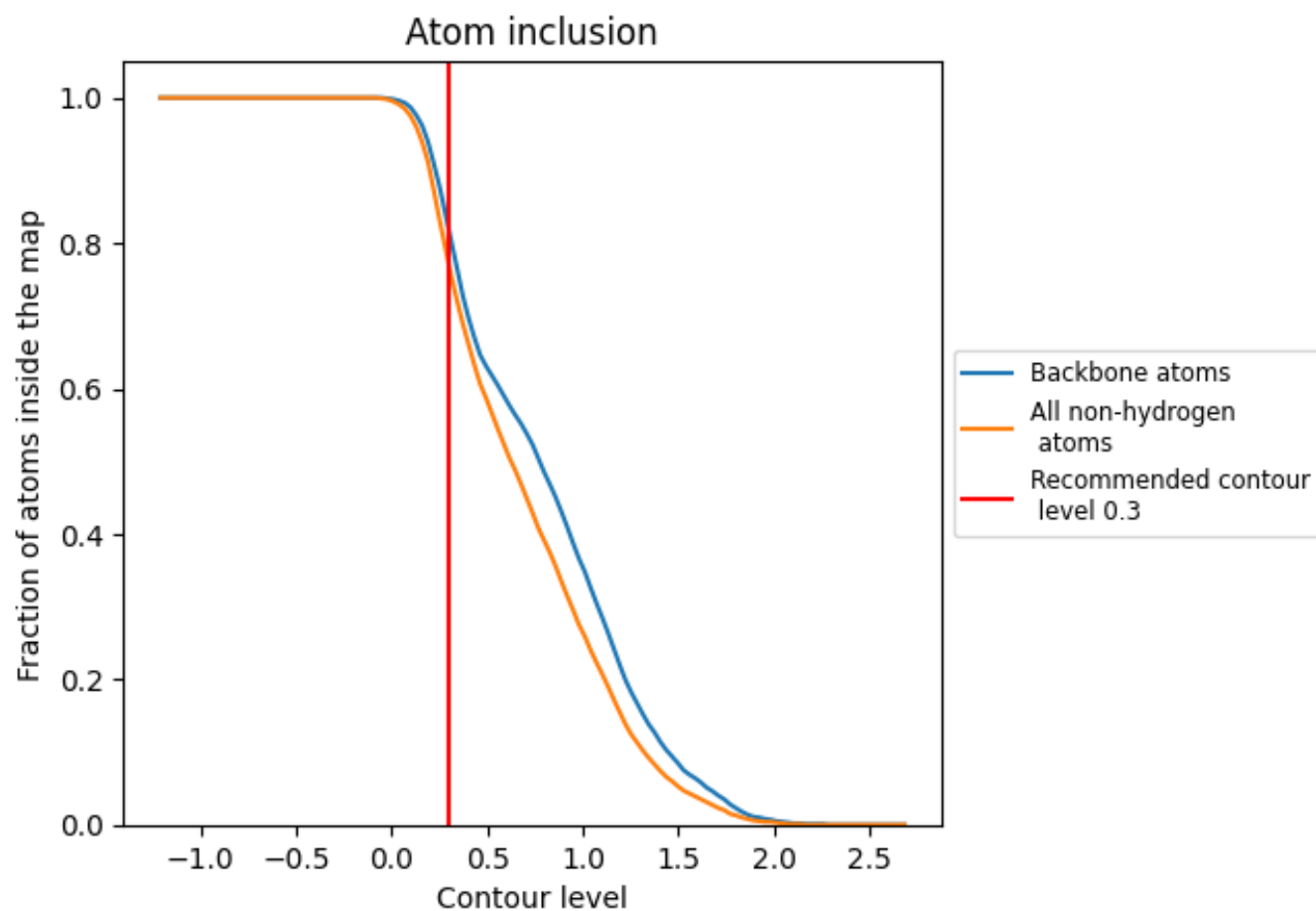
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.5220
A	 0.7690	 0.5260
B	 0.7700	 0.5200
C	 0.7670	 0.5240
D	 0.7670	 0.5220
E	 0.7650	 0.5150
F	 0.7680	 0.5250
G	 0.7680	 0.5210
H	 0.7660	 0.5200
I	 0.7690	 0.5250
J	 0.7710	 0.5220
K	 0.7720	 0.5220
L	 0.7700	 0.5250
M	 0.7660	 0.5180
N	 0.7590	 0.5150
O	 0.7670	 0.5220
P	 0.7670	 0.5190
Q	 0.7680	 0.5220
R	 0.7680	 0.5210
S	 0.7700	 0.5230
T	 0.7670	 0.5150
U	 0.7660	 0.5230
V	 0.7690	 0.5240
W	 0.7680	 0.5220
X	 0.7690	 0.5240

