



## wwPDB EM Validation Summary Report ⓘ

May 31, 2025 – 01:04 PM EDT

PDB ID : 9D93 / pdb\_00009d93  
EMDB ID : EMD-46661  
Title : Mycobacteriophage Bxb1 tail tip - Composite map and model  
Authors : Freeman, K.G.  
Deposited on : 2024-08-20  
Resolution : 2.85 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

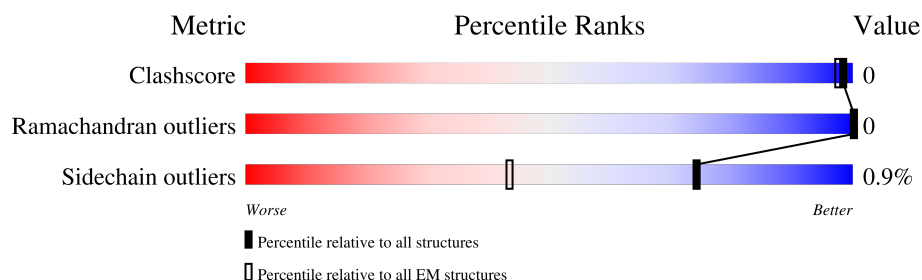
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













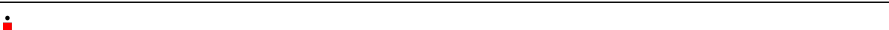

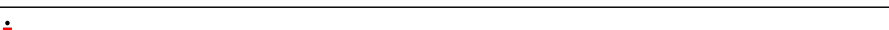
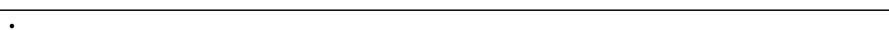
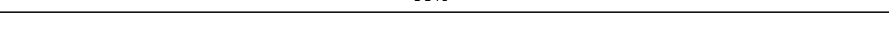
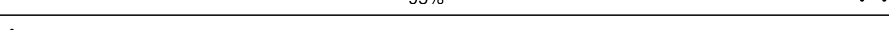
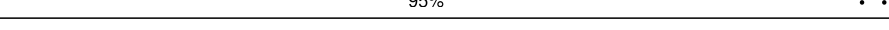
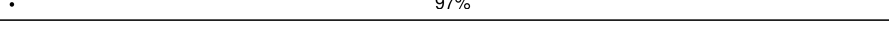
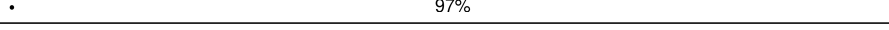
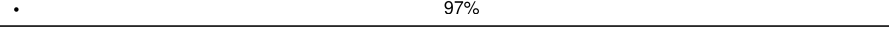
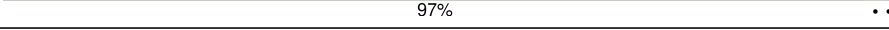
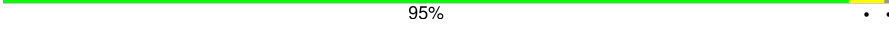
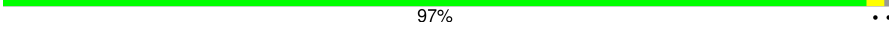
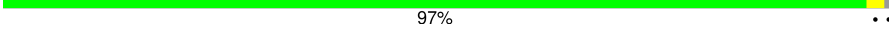
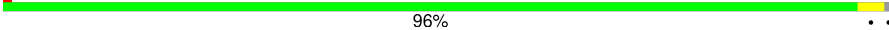
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	Ja	283	
1	Jb	283	
1	Jc	283	
1	Jd	283	
1	Je	283	
1	Jf	283	
2	Ka	86	
2	Kb	86	

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Mol	Chain	Length	Quality of chain
2	Kc	86	 93%
3	La	356	 29% 69%
3	Lb	356	 29% 69%
3	Lc	356	 30% 69%
3	Ld	356	 30% 69%
3	Le	356	 29% 69%
3	Lf	356	 29% 69%
3	Lg	356	 30% 69%
3	Lh	356	 30% 69%
3	Li	356	 30% 69%
4	Ma	685	 94%
4	Mb	685	 95%
4	Mc	685	 95%
4	Md	685	 96%
4	Me	685	 95%
4	Mf	685	 95%
5	Na	823	 97%
5	Nb	823	 97%
5	Nc	823	 97%
6	Oa	600	 97%
6	Ob	600	 95%
6	Oc	600	 97%
7	Pa	617	 97%
7	Pb	617	 96%
7	Pc	617	 98%

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Mol	Chain	Length	Quality of chain
8	Qa	267	
8	Qb	267	
8	Qc	267	
9	Ra	106	
9	Rb	106	
9	Rc	106	
9	Rd	106	
9	Re	106	
9	Rf	106	
10	Sa	496	
10	Sb	496	
10	Sc	496	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 199287 atoms, of which 97837 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 Tail tube, gp19.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ja	282	Total	C	H	N	O	0	0
			4163	1345	2039	344	435		
1	Jb	281	Total	C	H	N	O	0	0
			4146	1340	2030	343	433		
1	Jc	282	Total	C	H	N	O	0	0
			4163	1345	2039	344	435		
1	Jd	281	Total	C	H	N	O	0	0
			4146	1340	2030	343	433		
1	Je	282	Total	C	H	N	O	0	0
			4163	1345	2039	344	435		
1	Jf	282	Total	C	H	N	O	0	0
			4163	1345	2039	344	435		

- Molecule 2 is a protein called Tail collar spacer, gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ka	83	Total	C	H	N	O	0	0
			1294	415	634	116	129		
2	Kb	83	Total	C	H	N	O	0	0
			1294	415	634	116	129		
2	Kc	83	Total	C	H	N	O	0	0
			1294	415	634	116	129		

- Molecule 3 is a protein called Tail collar fibers, gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	La	109	Total	C	H	N	O	0	0
			1641	530	808	136	167		
3	Lb	110	Total	C	H	N	O	0	0
			1652	533	813	137	169		
3	Lc	109	Total	C	H	N	O	0	0
			1641	530	808	136	167		
3	Ld	110	Total	C	H	N	O	0	0
			1652	533	813	137	169		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Le	109	Total	C	H	N	O	0	0
			1641	530	808	136	167		
3	Lf	109	Total	C	H	N	O	0	0
			1641	530	808	136	167		
3	Lg	109	Total	C	H	N	O	0	0
			1641	530	808	136	167		
3	Lh	110	Total	C	H	N	O	0	0
			1652	533	813	137	169		
3	Li	110	Total	C	H	N	O	0	0
			1652	533	813	137	169		

- Molecule 4 is a protein called Tail tip cage, gp23.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ma	670	Total	C	H	N	O	S	0	0
			10106	3246	4965	862	1027	6		
4	Mb	670	Total	C	H	N	O	S	0	0
			10106	3246	4965	862	1027	6		
4	Mc	671	Total	C	H	N	O	S	0	0
			10118	3250	4969	863	1030	6		
4	Md	671	Total	C	H	N	O	S	0	0
			10117	3249	4970	863	1029	6		
4	Me	670	Total	C	H	N	O	S	0	0
			10104	3246	4963	862	1027	6		
4	Mf	671	Total	C	H	N	O	S	0	0
			10117	3250	4968	863	1030	6		

- Molecule 5 is a protein called Tapemeasure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Na	22	Total	C	H	N	O	0	0
			355	107	179	34	35		
5	Nb	22	Total	C	H	N	O	0	0
			355	107	179	34	35		
5	Nc	22	Total	C	H	N	O	0	0
			355	107	179	34	35		

- Molecule 6 is a protein called Baseplate hub, gp25.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Oa	595	Total	C	H	N	O	S	0	0
			9309	3043	4604	788	859	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	Ob	595	Total	C	H	N	O	S	0	0
			9308	3043	4603	788	859	15		
6	Oc	595	Total	C	H	N	O	S	0	0
			9308	3043	4603	788	859	15		

- Molecule 7 is a protein called Tail spike, gp29.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Pa	610	Total	C	H	N	O	S	0	0
			8827	2814	4361	760	884	8		
7	Pb	610	Total	C	H	N	O	S	0	0
			8826	2814	4360	760	884	8		
7	Pc	610	Total	C	H	N	O	S	0	0
			8826	2814	4360	760	884	8		

- Molecule 8 is a protein called Tail wing brush, gp33.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Qa	230	Total	C	H	N	O	S	0	0
			2808	862	1336	278	331	1		
8	Qb	229	Total	C	H	N	O	S	0	0
			2794	857	1329	277	330	1		
8	Qc	230	Total	C	H	N	O	S	0	0
			2808	862	1336	278	331	1		

- Molecule 9 is a protein called Tail wing arm, gp31.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Ra	105	Total	C	H	N	O		0	0
			1555	503	764	126	162			
9	Rb	105	Total	C	H	N	O		0	0
			1555	503	764	126	162			
9	Rc	105	Total	C	H	N	O		0	0
			1555	503	764	126	162			
9	Rd	105	Total	C	H	N	O		0	0
			1555	503	764	126	162			
9	Re	105	Total	C	H	N	O		0	0
			1555	503	764	126	162			
9	Rf	105	Total	C	H	N	O		0	0
			1555	503	764	126	162			

- Molecule 10 is a protein called Tail wing base, gp30.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	Sa	477	Total	C	H	N	O	S	0	0
			7279	2375	3550	613	725	16		
10	Sb	475	Total	C	H	N	O	S	0	0
			7246	2365	3532	611	722	16		
10	Sc	475	Total	C	H	N	O	S	0	0
			7246	2365	3532	611	722	16		

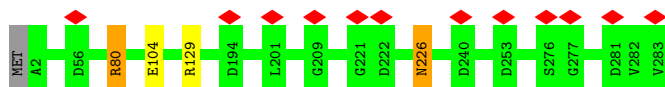


### 3 Residue-property plots [i](#)

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.

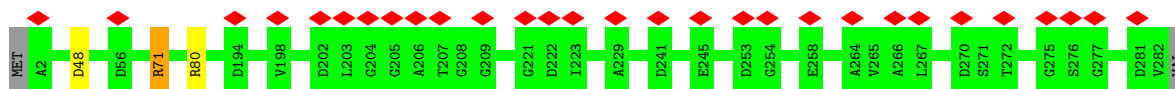
- Molecule 1: Tail tube, gp19

Chain Ja:  98%



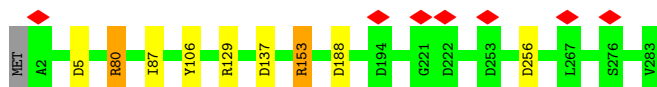
- Molecule 1: Tail tube, gp19

Chain Jb:  10% 98%



- Molecule 1: Tail tube, gp19

Chain Jc:  96%



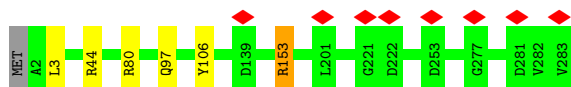
- Molecule 1: Tail tube, gp19

Chain Jd:  10% 96%



- Molecule 1: Tail tube, gp19

Chain Je:  98%





- Molecule 3: Tail collar fibers, gp4

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GLN	TYR	ALA	LEU	TRP	MET
THR	THR	CYS	ASN	ASP	T2
ALA	ALA	VAL	GLU	ASP	R10
ILE	ILE	GLY	LEU	ASP	R41
GLY	GLY	ASP	ALA	ASP	Y65
THR	THR	THR	ALA	LYS	L97
LYS	ARG	SER	LEU	PRO	F110
ASP	ASP	LEU	GLY	SER	SER
SER	SER	LEU	ASP	THR	ALA
ASN	ASN	ASN	ASP	PHE	THR
THR	THR	THR	PRO	THR	PRO
ALA	ALA	GLY	VAL	HIS	ASP
		SER	ALA	HIS	ALA
		SER	ALA	SER	LEU
		VAL	SER	ILE	SER
		THR	GLN	ALA	THR
		ASN	ILE	ASN	ALA
		ALA	GLY	VAL	VAL
		LYS	ALA	THR	PRO
		VAL	LYS	GLY	SER
		ALA	ALA	LEU	THR
		THR	THR	GLU	ASP
		ILE	THR	ASP	ALA
		ALA	ILE	GLU	ALA
		LEU	THR	LYS	ASP
		SER	ALA	HIS	VAL
		LYS	GLY	ASP	ALA
		LEU	THR	GLU	ALA
		VAL	GLY	GLY	VAL
		VAL	GLY	ASP	THR
		ALA	GLY	ALA	THR
		GLY	GLY	ARG	ALA
		SER	ASP	VAL	THR
		THR	LEU	SER	ALA
		ASP	SER	LEU	THR
		ASN	ALA	GLY	ALA
		SER	ASN	THR	TTR
		GLY	ARG	ALA	LEU
		ALA	THR	ALA	ALA
		THR	THR	LEU	VAL
		THR	ASN	VAL	SER
		ILE	SER	ASN	THR
		THR	PHE	ALA	PRO
		TRP	GLY	PRO	GLU
		VAL	THR	THR	ALA
		GLY	SER	THR	GLY
		THR	SER	LEU	SER
		GLU	THR	ASP	VAL
		ALA	THR	THR	ALA

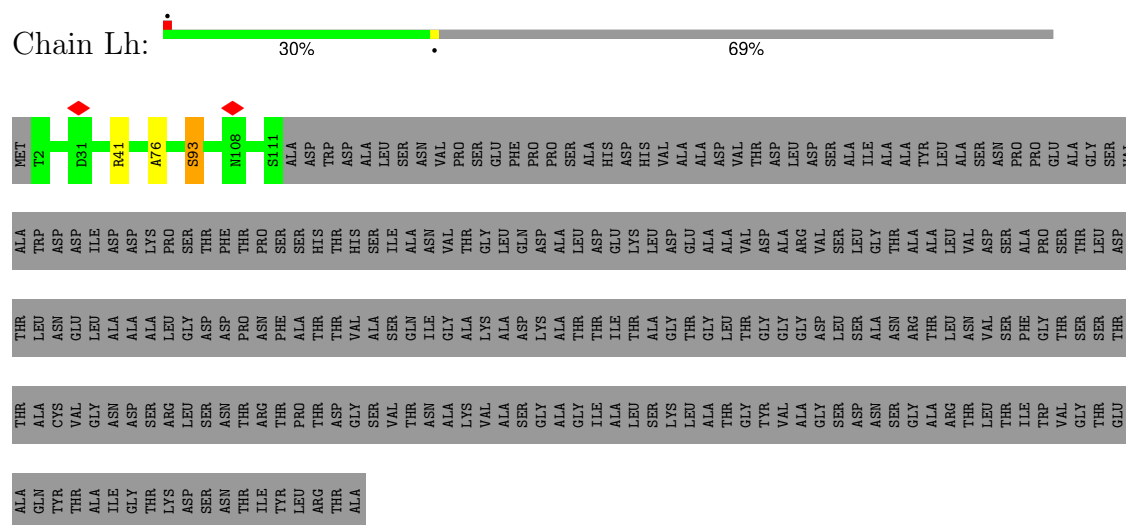
Chain Lf:  29% 69%

[illegible]

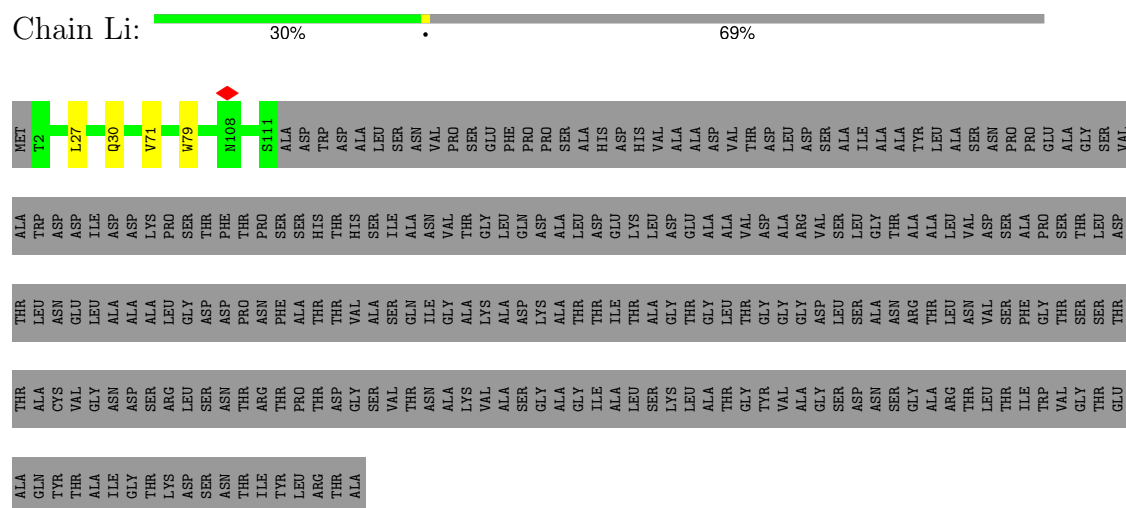
Chain Lg:  30% 69%

[illegible]

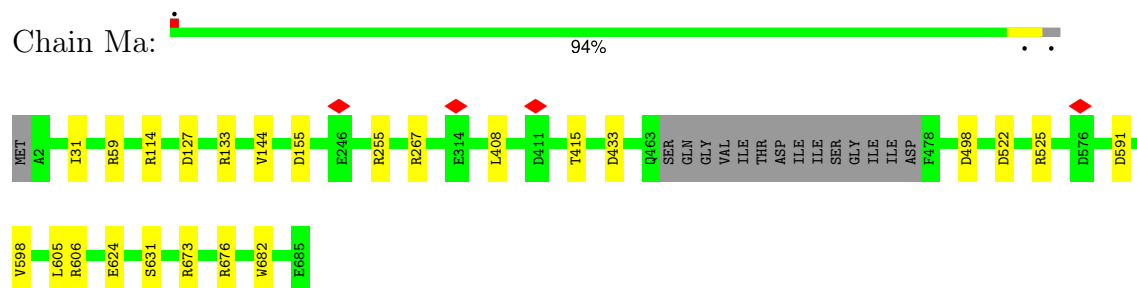
- Molecule 3: Tail collar fibers, gp4



- Molecule 3: Tail collar fibers, gp4

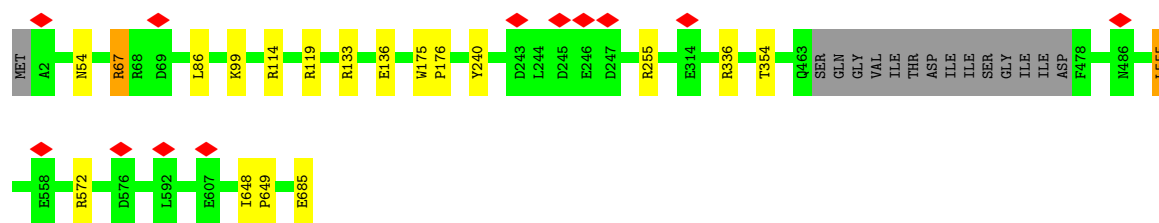


- Molecule 4: Tail tip cage, gp23



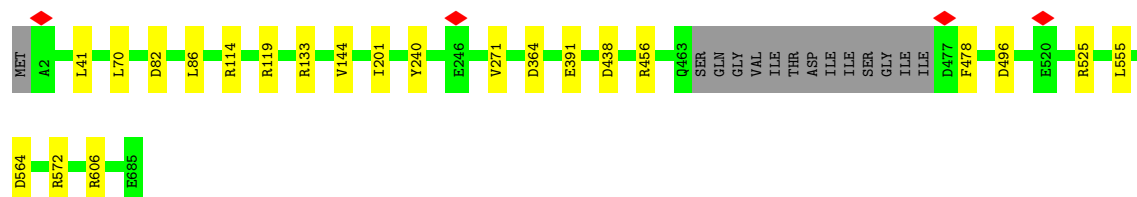
- Molecule 4: Tail tip cage, gp23





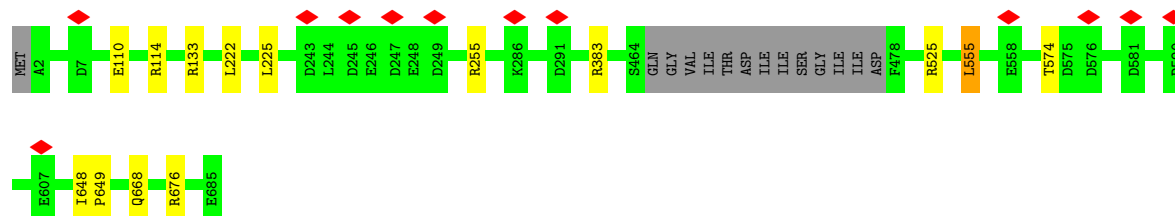
- Molecule 4: Tail tip cage, gp23

Chain Mc: 95%



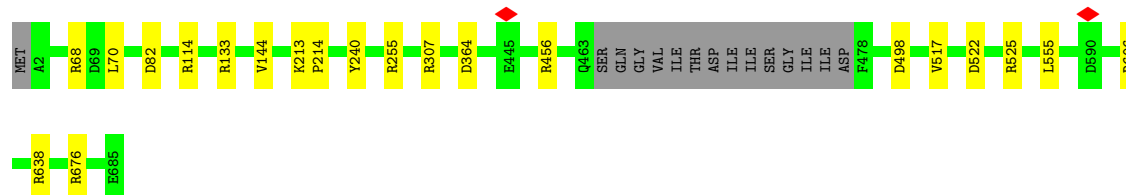
- Molecule 4: Tail tip cage, gp23

Chain Md: 96%



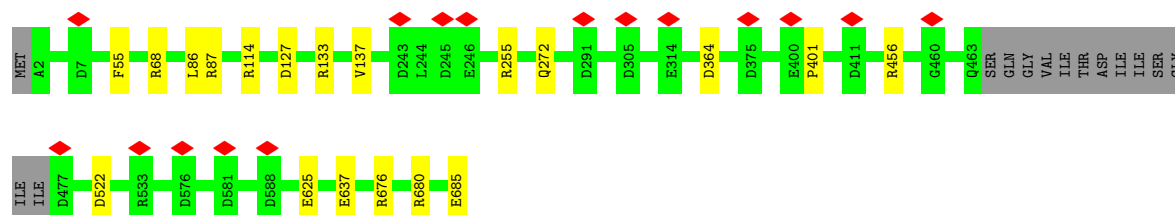
- Molecule 4: Tail tip cage, gp23

Chain Me: 95%

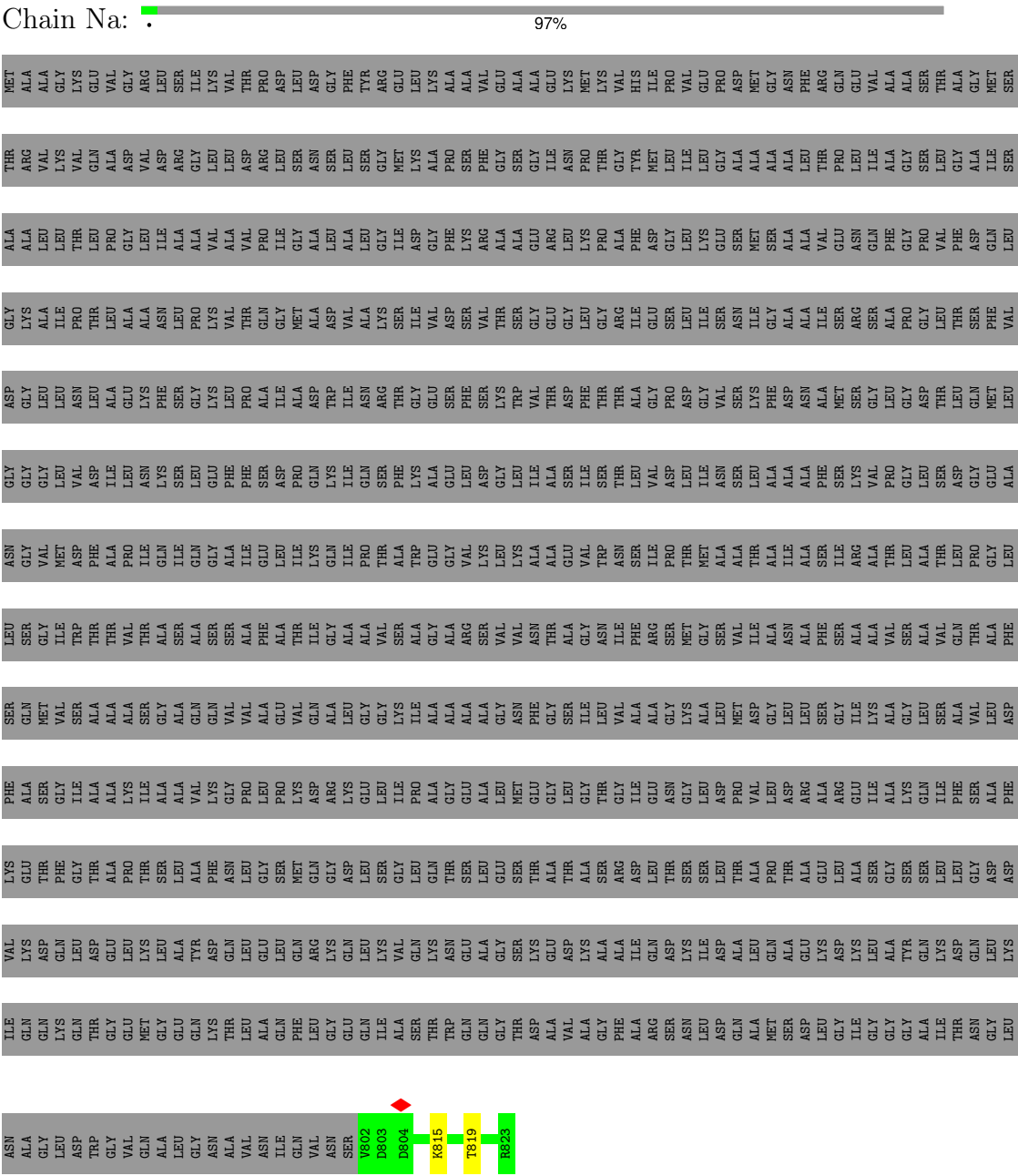


- Molecule 4: Tail tip cage, gp23

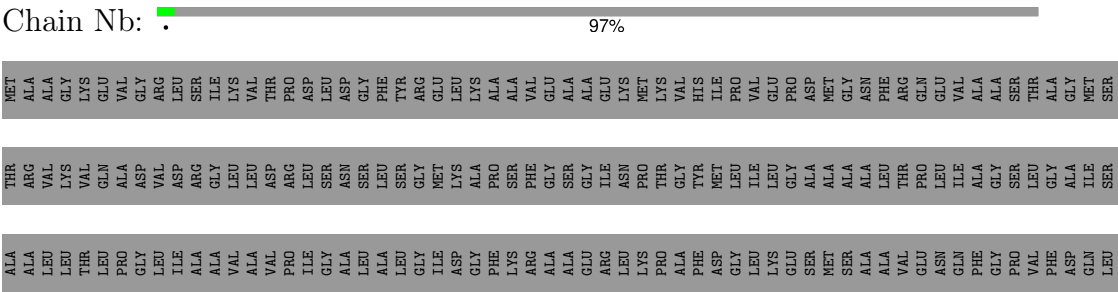
Chain Mf: 95%



● Molecule 5: Tapemeasure protein



● Molecule 5: Tapemeasure protein







ASN	V802
ALA	D803
GLY	D804
LEU	
ASP	
TRP	
GLY	
VAL	
GLN	
ALA	
LEU	
GLY	
ASN	
ALA	
VAL	
ASN	
ILE	
GLN	
VAL	
ASN	
SER	
	R822
	R823

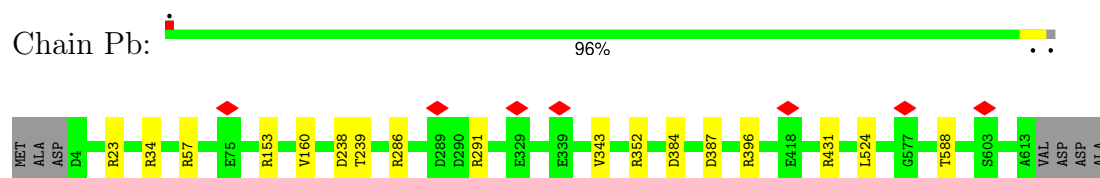
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|-----|--|----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|
| MET |  | A5 | R25 | L37 | Y45 | I83 | R92 | R108 | M109 | R116 | V122 | T245 | R311 | E357 | E577 | I580 | I599 | LEU |
|-----|--|----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|

- | MET  | PRO  | ALA  | PRO  |
|------|------|------|------|
| A5   | R25  | D44  | R48  |
|      |      | R55  | R92  |
|      | H95  | R108 | R116 |
|      | E125 | R248 | E265 |
| I271 | R311 | A312 | V313 |
|      | A317 | S318 | D319 |
| T322 |      |      |      |
| V360 | D375 | N397 | L406 |
|      | D514 | Y541 | P542 |
|      |      | D543 | K565 |
|      |      |      | I599 |

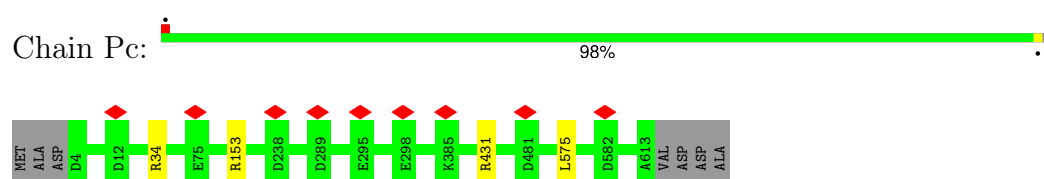
- |      |
|------|
| MET  |
| PRO  |
| ALA  |
| PRO  |
| A5   |
| Q26  |
| Y45  |
| R43  |
| T66  |
| S70  |
| H95  |
| R108 |
| E265 |
| R311 |
| L406 |
| R435 |
| R496 |
| R523 |
| E575 |
| P576 |
| E577 |
| I59  |
| LEU  |

- [illegible]

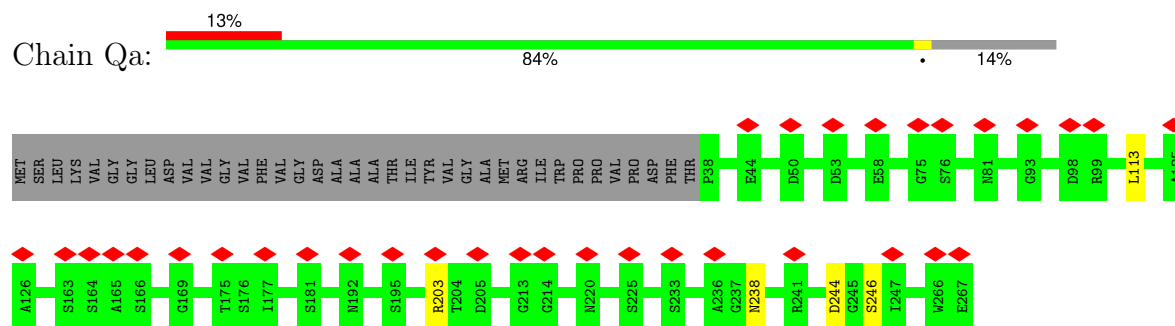
- Molecule 7: Tail spike, gp29



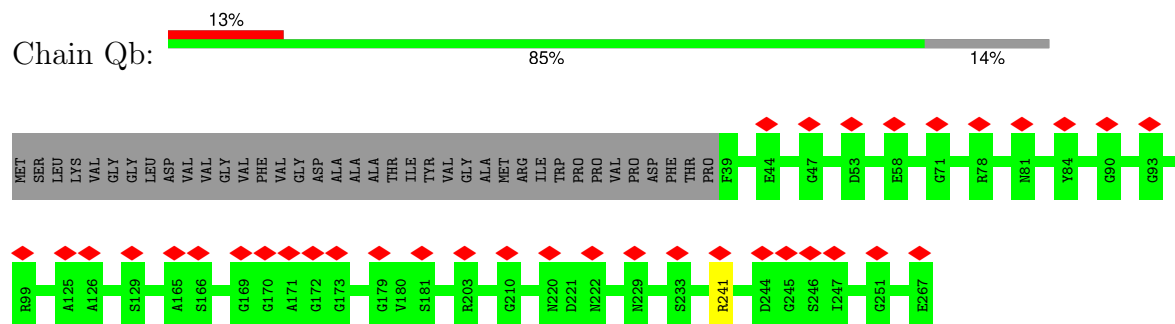
- Molecule 7: Tail spike, gp29



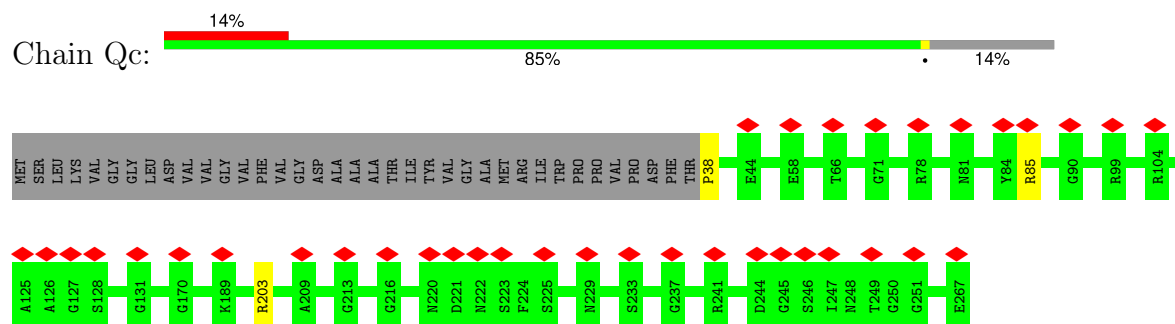
- Molecule 8: Tail wing brush, gp33



- Molecule 8: Tail wing brush, gp33



- Molecule 8: Tail wing brush, gp33



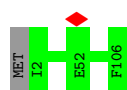
- Molecule 9: Tail wing arm, gp31

Chain Ra:  99%



- Molecule 9: Tail wing arm, gp31

Chain Rb:  99%



- Molecule 9: Tail wing arm, gp31

Chain Rc:  98%



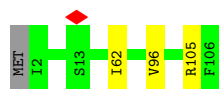
- Molecule 9: Tail wing arm, gp31

Chain Rd:  96%



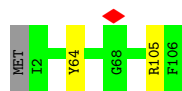
- Molecule 9: Tail wing arm, gp31

Chain Re:  96%



- Molecule 9: Tail wing arm, gp31

Chain Rf:  97%



- Molecule 10: Tail wing base, gp30

Chain Sa:  94%

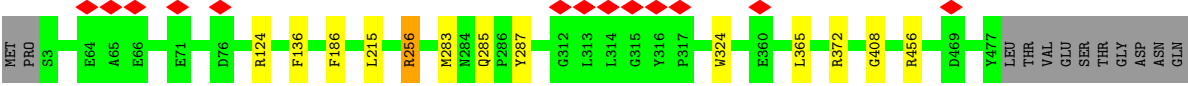


ASN  
GLN  
ILE  
PRO  
ALA  
ASP  
VAL  
PRO  
PHE  
GLU  
ILE

● Molecule 10: Tail wing base, gp30



● Molecule 10: Tail wing base, gp30



ILE  
PRO  
ALA  
ASP  
VAL  
PRO  
PHE  
GLU  
ILE

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22280	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.051	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	Ja	0.69	0/2167	1.26	3/2958 (0.1%)
1	Jb	0.71	0/2159	1.27	3/2948 (0.1%)
1	Jc	0.68	0/2167	1.25	6/2958 (0.2%)
1	Jd	0.72	0/2159	1.30	7/2948 (0.2%)
1	Je	0.70	0/2167	1.27	4/2958 (0.1%)
1	Jf	0.72	0/2167	1.28	4/2958 (0.1%)
2	Ka	0.75	0/678	1.31	0/932
2	Kb	0.75	0/678	1.34	0/932
2	Kc	0.73	0/678	1.33	2/932 (0.2%)
3	La	0.68	0/852	1.27	1/1174 (0.1%)
3	Lb	0.70	0/858	1.28	4/1182 (0.3%)
3	Lc	0.71	0/852	1.30	1/1174 (0.1%)
3	Ld	0.70	0/858	1.29	3/1182 (0.3%)
3	Le	0.67	0/852	1.25	2/1174 (0.2%)
3	Lf	0.68	0/852	1.29	1/1174 (0.1%)
3	Lg	0.68	0/852	1.27	1/1174 (0.1%)
3	Lh	0.72	0/858	1.34	3/1182 (0.3%)
3	Li	0.72	0/858	1.35	0/1182
4	Ma	0.74	0/5265	1.31	10/7203 (0.1%)
4	Mb	0.72	0/5265	1.27	9/7203 (0.1%)
4	Mc	0.74	0/5273	1.30	7/7214 (0.1%)
4	Md	0.73	0/5271	1.28	9/7211 (0.1%)
4	Me	0.74	0/5265	1.29	5/7203 (0.1%)
4	Mf	0.73	0/5273	1.30	12/7214 (0.2%)
5	Na	0.76	0/176	1.38	0/237
5	Nb	0.74	0/176	1.34	0/237
5	Nc	0.73	0/176	1.38	0/237
6	Oa	0.73	0/4844	1.32	5/6597 (0.1%)
6	Ob	0.72	0/4844	1.34	16/6597 (0.2%)
6	Oc	0.72	0/4844	1.34	7/6597 (0.1%)
7	Pa	0.70	0/4563	1.33	8/6227 (0.1%)
7	Pb	0.70	0/4563	1.33	11/6227 (0.2%)
7	Pc	0.69	0/4563	1.32	3/6227 (0.0%)
8	Qa	0.77	0/1494	1.34	2/2006 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	Qb	0.75	0/1486	1.30	1/1995 (0.1%)
8	Qc	0.74	0/1494	1.32	3/2006 (0.1%)
9	Ra	0.71	0/811	1.26	0/1114
9	Rb	0.71	0/811	1.26	0/1114
9	Rc	0.71	0/811	1.24	1/1114 (0.1%)
9	Rd	0.77	0/811	1.29	1/1114 (0.1%)
9	Re	0.73	0/811	1.29	1/1114 (0.1%)
9	Rf	0.75	0/811	1.28	1/1114 (0.1%)
10	Sa	0.71	0/3831	1.30	4/5228 (0.1%)
10	Sb	0.71	0/3816	1.29	5/5207 (0.1%)
10	Sc	0.71	0/3816	1.30	7/5207 (0.1%)
All	All	0.72	0/103876	1.30	173/141886 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ja	0	1
1	Jc	0	2
1	Jd	0	1
1	Je	0	1
3	La	0	1
3	Lb	0	1
3	Lc	0	1
3	Ld	0	1
3	Le	0	2
3	Lf	0	2
3	Lg	0	1
4	Ma	0	3
4	Mb	0	3
4	Mc	0	4
4	Me	0	5
5	Nc	0	1
6	Oc	0	1
7	Pa	0	1
7	Pb	0	2
9	Rd	0	1
9	Rf	0	1
10	Sa	0	1
10	Sb	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	Sc	0	1
All	All	0	39

There are no bond length outliers.

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Mf	133	ARG	NE-CZ-NH2	6.88	125.39	119.20
6	Ob	55	ARG	NE-CZ-NH2	6.78	125.31	119.20
4	Me	133	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	Jc	129	ARG	NE-CZ-NH2	6.60	125.14	119.20
6	Oc	95	HIS	CB-CG-CD2	-6.56	122.67	131.20

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Ja	80	ARG	Sidechain
1	Jc	153	ARG	Sidechain
1	Jc	80	ARG	Sidechain
1	Jd	170	ARG	Sidechain
1	Je	153	ARG	Sidechain

## 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	Ja	2124	2039	2038	0	0
1	Jb	2116	2030	2029	1	0
1	Jc	2124	2039	2038	1	0
1	Jd	2116	2030	2029	0	0
1	Je	2124	2039	2038	1	0
1	Jf	2124	2039	2038	0	0
2	Ka	660	634	633	0	0
2	Kb	660	634	633	0	0
2	Kc	660	634	633	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	La	833	808	807	0	0
3	Lb	839	813	812	0	0
3	Lc	833	808	807	0	0
3	Ld	839	813	812	1	0
3	Le	833	808	807	0	0
3	Lf	833	808	807	0	0
3	Lg	833	808	807	0	0
3	Lh	839	813	812	0	0
3	Li	839	813	812	1	0
4	Ma	5141	4965	4963	2	0
4	Mb	5141	4965	4963	3	0
4	Mc	5149	4969	4967	4	0
4	Md	5147	4970	4968	2	0
4	Me	5141	4963	4963	1	0
4	Mf	5149	4968	4967	3	0
5	Na	176	179	178	1	0
5	Nb	176	179	178	1	0
5	Nc	176	179	178	0	0
6	Oa	4705	4604	4602	2	0
6	Ob	4705	4603	4602	2	0
6	Oc	4705	4603	4602	2	0
7	Pa	4466	4361	4359	1	0
7	Pb	4466	4360	4359	0	0
7	Pc	4466	4360	4359	0	0
8	Qa	1472	1336	1336	1	0
8	Qb	1465	1329	1328	0	0
8	Qc	1472	1336	1336	0	0
9	Ra	791	764	763	0	0
9	Rb	791	764	763	0	0
9	Rc	791	764	763	0	0
9	Rd	791	764	763	0	0
9	Re	791	764	763	0	0
9	Rf	791	764	763	0	0
10	Sa	3729	3550	3549	2	0
10	Sb	3714	3532	3531	1	0
10	Sc	3714	3532	3531	3	0
All	All	101450	97837	97789	31	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 0.

The worst 5 of 31 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)
4:Ma:408:LEU:H	4:Ma:415:THR:HG22	1.73	0.54
10:Sa:388:MET:HE3	10:Sa:397:TRP:HB2	1.91	0.53
6:Oa:83:ILE:HG23	6:Oa:109:MET:HE1	1.90	0.53
4:Mb:555:LEU:H	4:Mb:555:LEU:HD22	1.75	0.52
1:Jb:71:ARG:HG3	4:Mf:137:VAL:HG21	1.92	0.51

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	Ja	280/283 (99%)	268 (96%)	12 (4%)	0	100	100
1	Jb	279/283 (99%)	268 (96%)	11 (4%)	0	100	100
1	Jc	280/283 (99%)	268 (96%)	12 (4%)	0	100	100
1	Jd	279/283 (99%)	267 (96%)	12 (4%)	0	100	100
1	Je	280/283 (99%)	265 (95%)	15 (5%)	0	100	100
1	Jf	280/283 (99%)	272 (97%)	8 (3%)	0	100	100
2	Ka	81/86 (94%)	78 (96%)	3 (4%)	0	100	100
2	Kb	81/86 (94%)	78 (96%)	3 (4%)	0	100	100
2	Kc	81/86 (94%)	80 (99%)	1 (1%)	0	100	100
3	La	107/356 (30%)	104 (97%)	3 (3%)	0	100	100
3	Lb	108/356 (30%)	107 (99%)	1 (1%)	0	100	100
3	Lc	107/356 (30%)	103 (96%)	4 (4%)	0	100	100
3	Ld	108/356 (30%)	104 (96%)	4 (4%)	0	100	100
3	Le	107/356 (30%)	104 (97%)	3 (3%)	0	100	100
3	Lf	107/356 (30%)	102 (95%)	5 (5%)	0	100	100
3	Lg	107/356 (30%)	102 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Lh	108/356 (30%)	104 (96%)	4 (4%)	0	100	100
3	Li	108/356 (30%)	103 (95%)	5 (5%)	0	100	100
4	Ma	666/685 (97%)	636 (96%)	30 (4%)	0	100	100
4	Mb	666/685 (97%)	640 (96%)	26 (4%)	0	100	100
4	Mc	667/685 (97%)	629 (94%)	38 (6%)	0	100	100
4	Md	667/685 (97%)	632 (95%)	35 (5%)	0	100	100
4	Me	666/685 (97%)	627 (94%)	39 (6%)	0	100	100
4	Mf	667/685 (97%)	637 (96%)	30 (4%)	0	100	100
5	Na	20/823 (2%)	20 (100%)	0	0	100	100
5	Nb	20/823 (2%)	20 (100%)	0	0	100	100
5	Nc	20/823 (2%)	20 (100%)	0	0	100	100
6	Oa	593/600 (99%)	578 (98%)	15 (2%)	0	100	100
6	Ob	593/600 (99%)	575 (97%)	18 (3%)	0	100	100
6	Oc	593/600 (99%)	583 (98%)	10 (2%)	0	100	100
7	Pa	608/617 (98%)	590 (97%)	18 (3%)	0	100	100
7	Pb	608/617 (98%)	584 (96%)	24 (4%)	0	100	100
7	Pc	608/617 (98%)	586 (96%)	22 (4%)	0	100	100
8	Qa	228/267 (85%)	220 (96%)	8 (4%)	0	100	100
8	Qb	227/267 (85%)	216 (95%)	11 (5%)	0	100	100
8	Qc	228/267 (85%)	224 (98%)	4 (2%)	0	100	100
9	Ra	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
9	Rb	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
9	Rc	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
9	Rd	103/106 (97%)	95 (92%)	8 (8%)	0	100	100
9	Re	103/106 (97%)	95 (92%)	8 (8%)	0	100	100
9	Rf	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
10	Sa	475/496 (96%)	456 (96%)	19 (4%)	0	100	100
10	Sb	473/496 (95%)	450 (95%)	23 (5%)	0	100	100
10	Sc	473/496 (95%)	455 (96%)	18 (4%)	0	100	100
All	All	13272/18315 (72%)	12738 (96%)	534 (4%)	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	Ja	220/221 (100%)	218 (99%)	2 (1%)	75	88
1	Jb	219/221 (99%)	219 (100%)	0	100	100
1	Jc	220/221 (100%)	219 (100%)	1 (0%)	86	94
1	Jd	219/221 (99%)	217 (99%)	2 (1%)	75	88
1	Je	220/221 (100%)	220 (100%)	0	100	100
1	Jf	220/221 (100%)	216 (98%)	4 (2%)	54	76
2	Ka	75/78 (96%)	75 (100%)	0	100	100
2	Kb	75/78 (96%)	74 (99%)	1 (1%)	65	83
2	Kc	75/78 (96%)	74 (99%)	1 (1%)	65	83
3	La	91/278 (33%)	89 (98%)	2 (2%)	47	71
3	Lb	92/278 (33%)	89 (97%)	3 (3%)	33	59
3	Lc	91/278 (33%)	91 (100%)	0	100	100
3	Ld	92/278 (33%)	92 (100%)	0	100	100
3	Le	91/278 (33%)	90 (99%)	1 (1%)	70	85
3	Lf	91/278 (33%)	89 (98%)	2 (2%)	47	71
3	Lg	91/278 (33%)	91 (100%)	0	100	100
3	Lh	92/278 (33%)	91 (99%)	1 (1%)	70	85
3	Li	92/278 (33%)	89 (97%)	3 (3%)	33	59
4	Ma	555/568 (98%)	547 (99%)	8 (1%)	62	82
4	Mb	555/568 (98%)	550 (99%)	5 (1%)	75	88
4	Mc	556/568 (98%)	550 (99%)	6 (1%)	70	85
4	Md	556/568 (98%)	551 (99%)	5 (1%)	75	88
4	Me	555/568 (98%)	546 (98%)	9 (2%)	58	79
4	Mf	556/568 (98%)	551 (99%)	5 (1%)	75	88
5	Na	19/613 (3%)	18 (95%)	1 (5%)	19	38
5	Nb	19/613 (3%)	18 (95%)	1 (5%)	19	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Nc	19/613 (3%)	18 (95%)	1 (5%)	19	38
6	Oa	496/500 (99%)	492 (99%)	4 (1%)	79	90
6	Ob	496/500 (99%)	490 (99%)	6 (1%)	67	84
6	Oc	496/500 (99%)	492 (99%)	4 (1%)	79	90
7	Pa	464/469 (99%)	460 (99%)	4 (1%)	75	88
7	Pb	464/469 (99%)	459 (99%)	5 (1%)	70	85
7	Pc	464/469 (99%)	463 (100%)	1 (0%)	92	97
8	Qa	137/165 (83%)	135 (98%)	2 (2%)	60	81
8	Qb	136/165 (82%)	136 (100%)	0	100	100
8	Qc	137/165 (83%)	137 (100%)	0	100	100
9	Ra	89/90 (99%)	89 (100%)	0	100	100
9	Rb	89/90 (99%)	89 (100%)	0	100	100
9	Rc	89/90 (99%)	89 (100%)	0	100	100
9	Rd	89/90 (99%)	87 (98%)	2 (2%)	47	71
9	Re	89/90 (99%)	87 (98%)	2 (2%)	47	71
9	Rf	89/90 (99%)	89 (100%)	0	100	100
10	Sa	391/408 (96%)	387 (99%)	4 (1%)	73	87
10	Sb	389/408 (95%)	388 (100%)	1 (0%)	91	96
10	Sc	389/408 (95%)	387 (100%)	2 (0%)	86	94
All	All	10749/14475 (74%)	10648 (99%)	101 (1%)	74	88

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Mf	364	ASP
6	Ob	271	ILE
10	Sc	215	LEU
4	Mf	637	GLU
6	Oa	45	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
5	Nb	816	GLN

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Mol	Chain	Res	Type
7	Pc	283	ASN
10	Sc	285	GLN
6	Oa	86	HIS
7	Pb	72	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](#)

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.

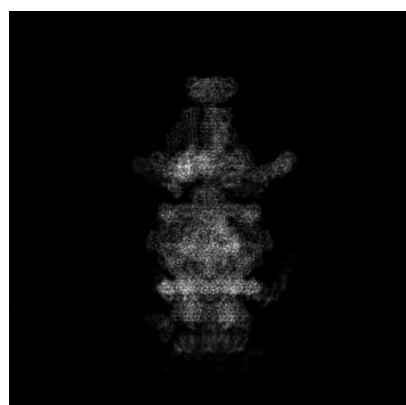
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46661. These allow visual inspection of the internal detail of the map and identification of artifacts.

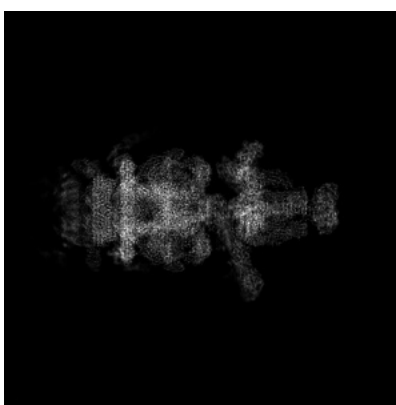
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

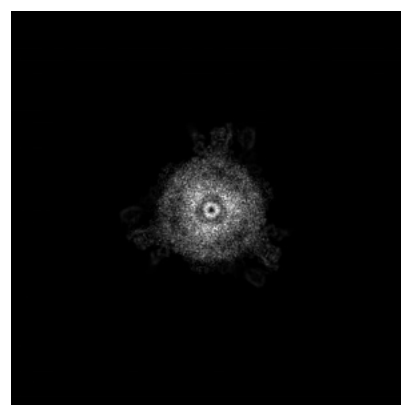
#### 6.1.1 Primary map



X



Y



Z

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

### 6.2 Central slices [i](#)

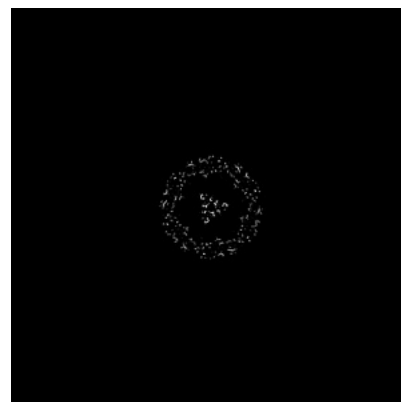
#### 6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

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

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

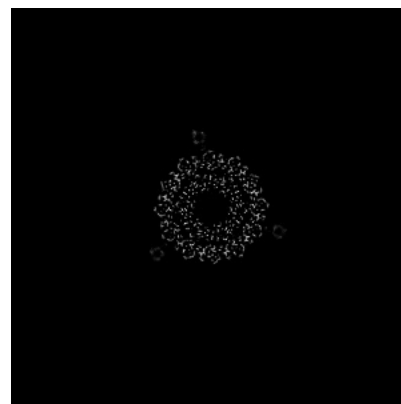
### 6.3.1 Primary map



X Index: 236



Y Index: 246

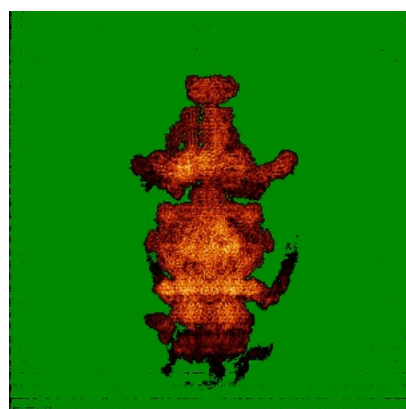


Z Index: 147

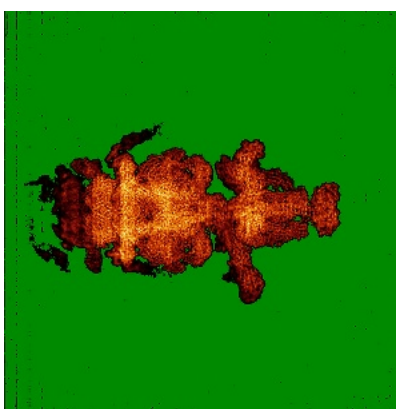
The images above show the largest variance slices of the map in three orthogonal directions.

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

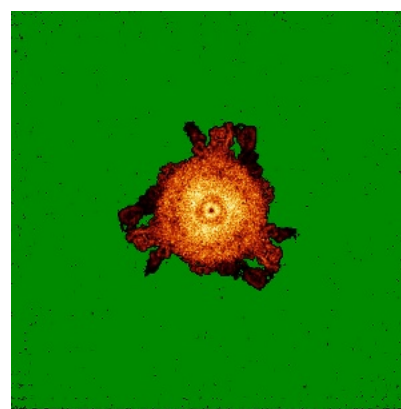
### 6.4.1 Primary map



X



Y



Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

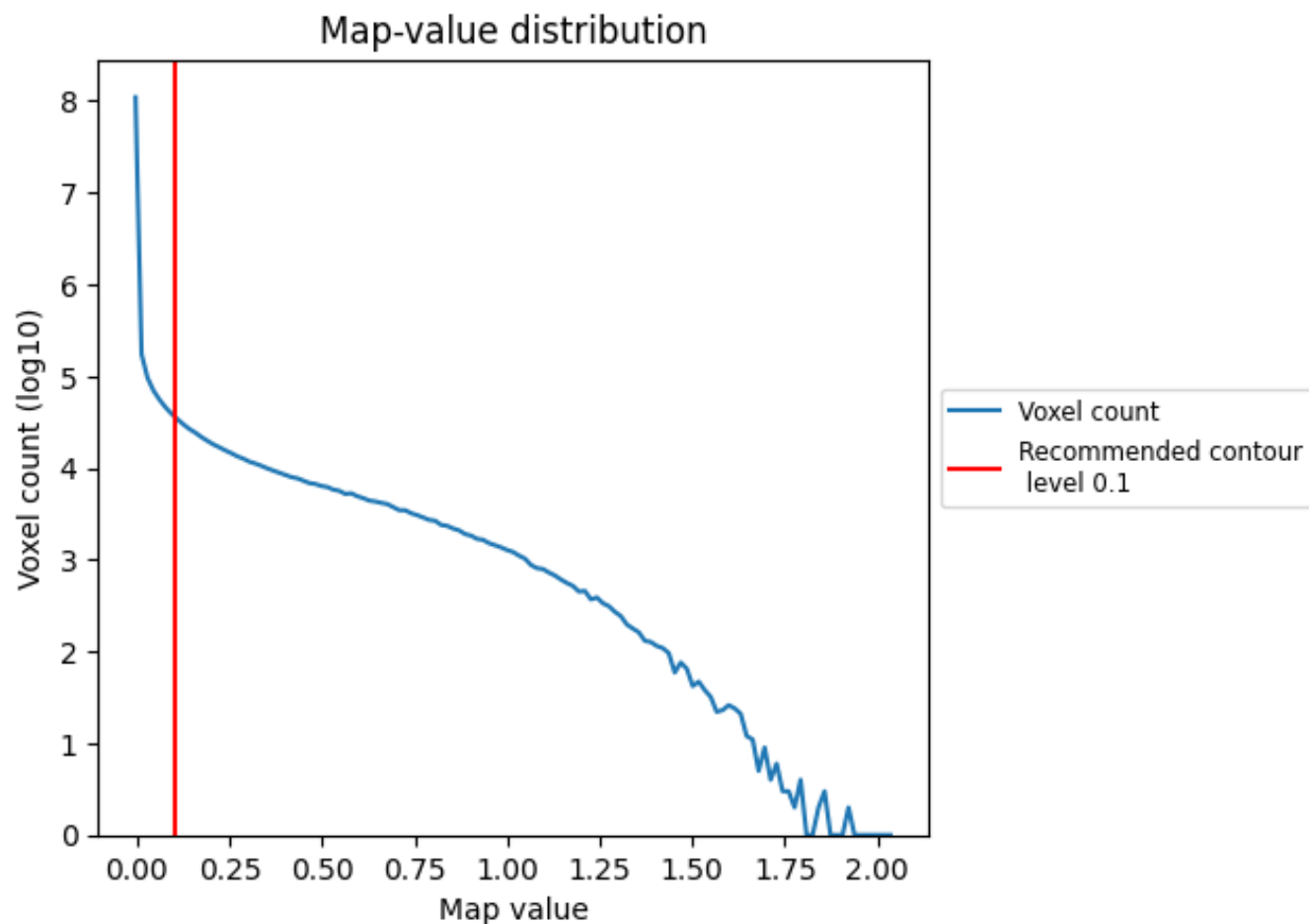
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

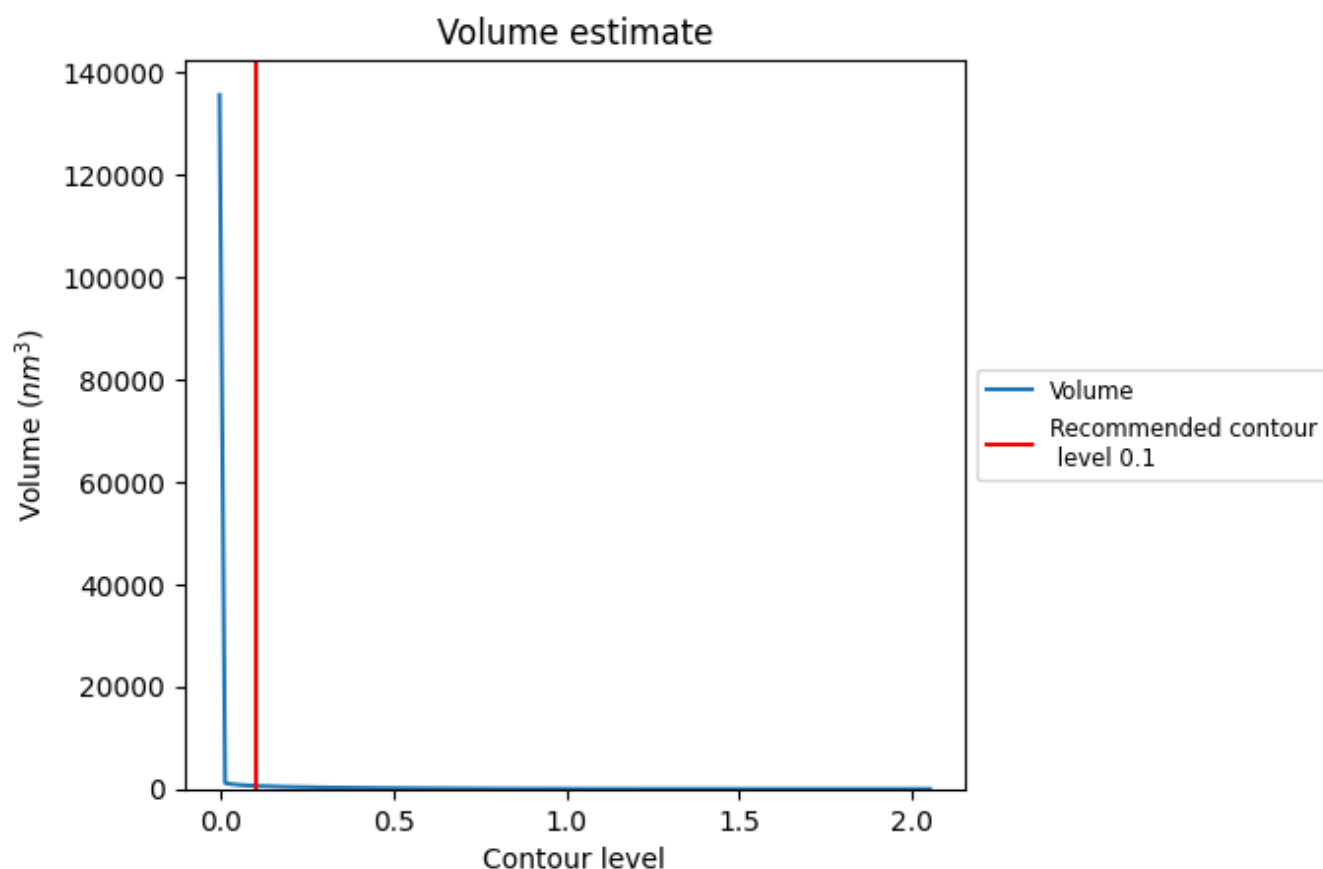
This section contains the results of statistical analysis of the map.

### 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.

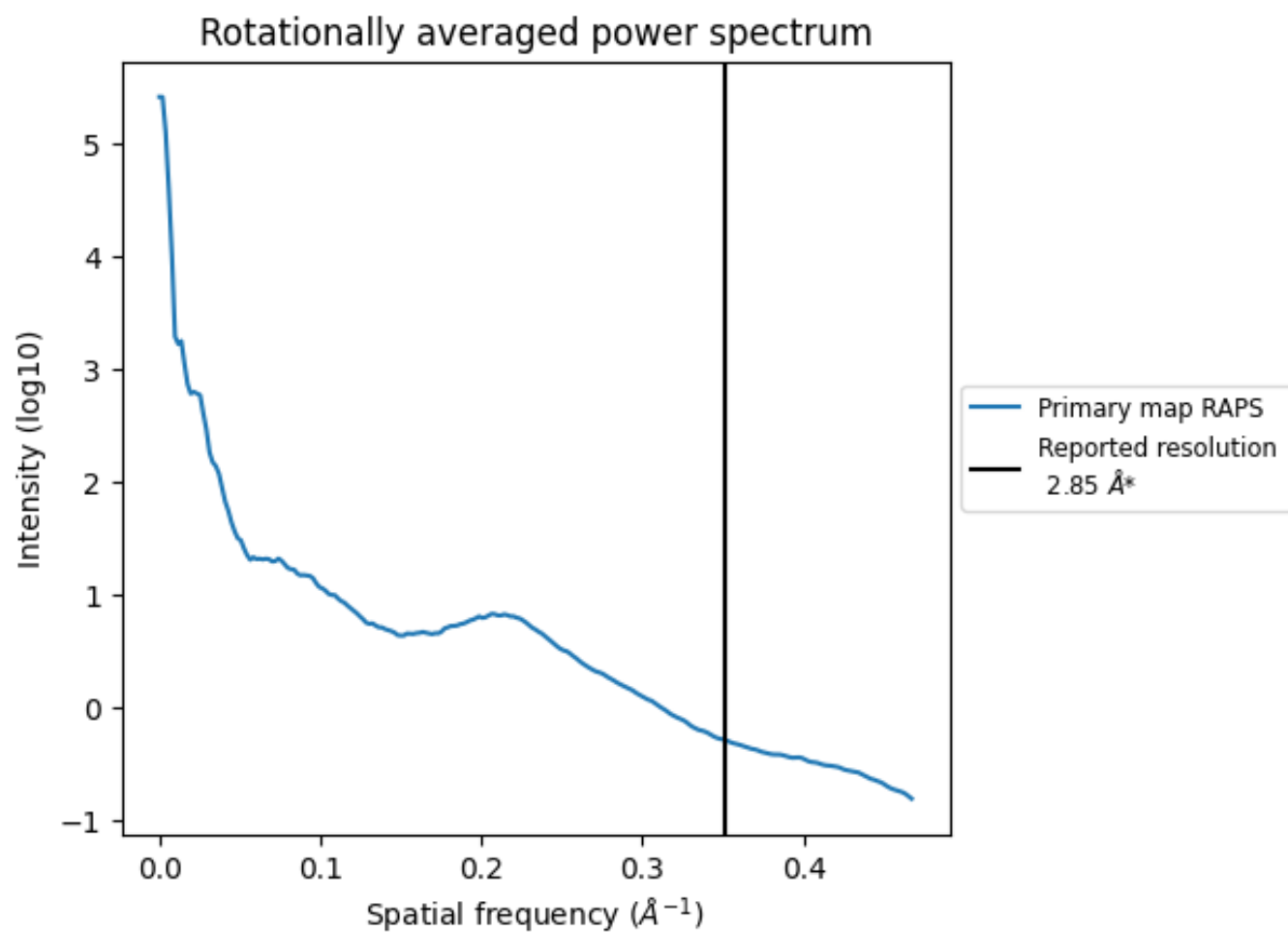
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 610  $\text{nm}^3$ ; this corresponds to an approximate mass of 551 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 0.351 Å<sup>-1</sup>

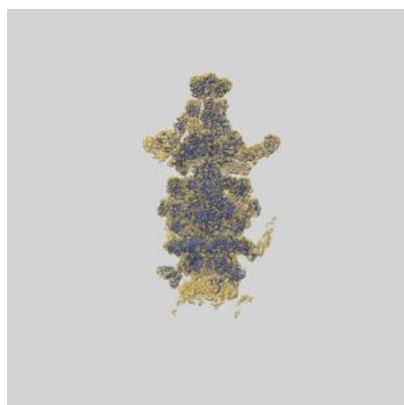
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

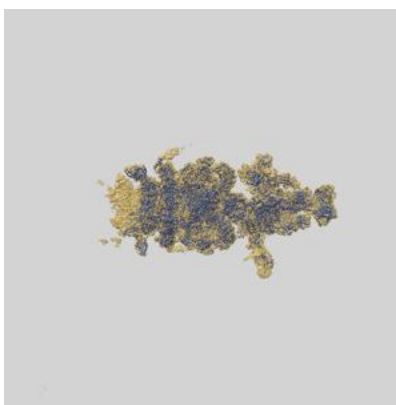
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46661 and PDB model 9D93. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

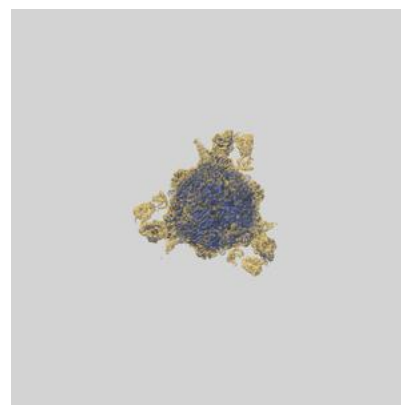
### 9.1 Map-model overlay [i](#)



X



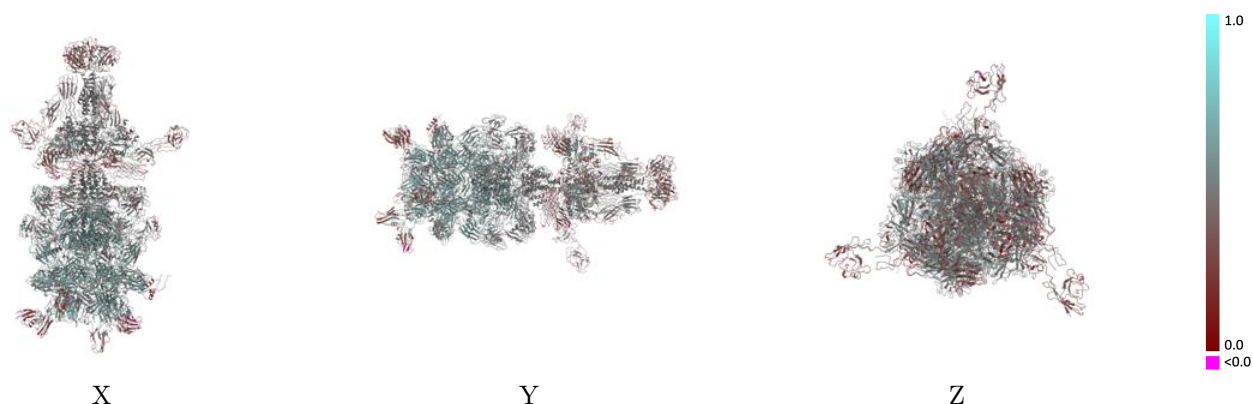
Y



Z

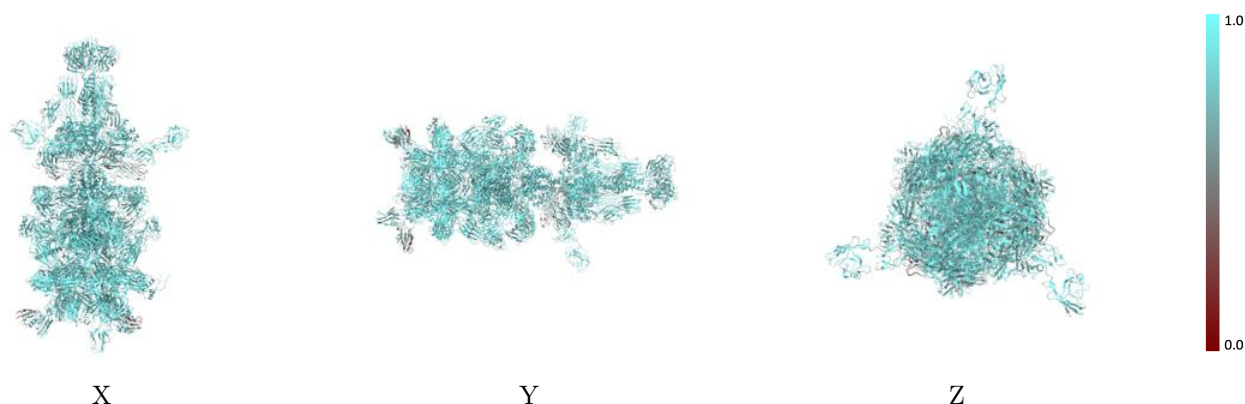
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



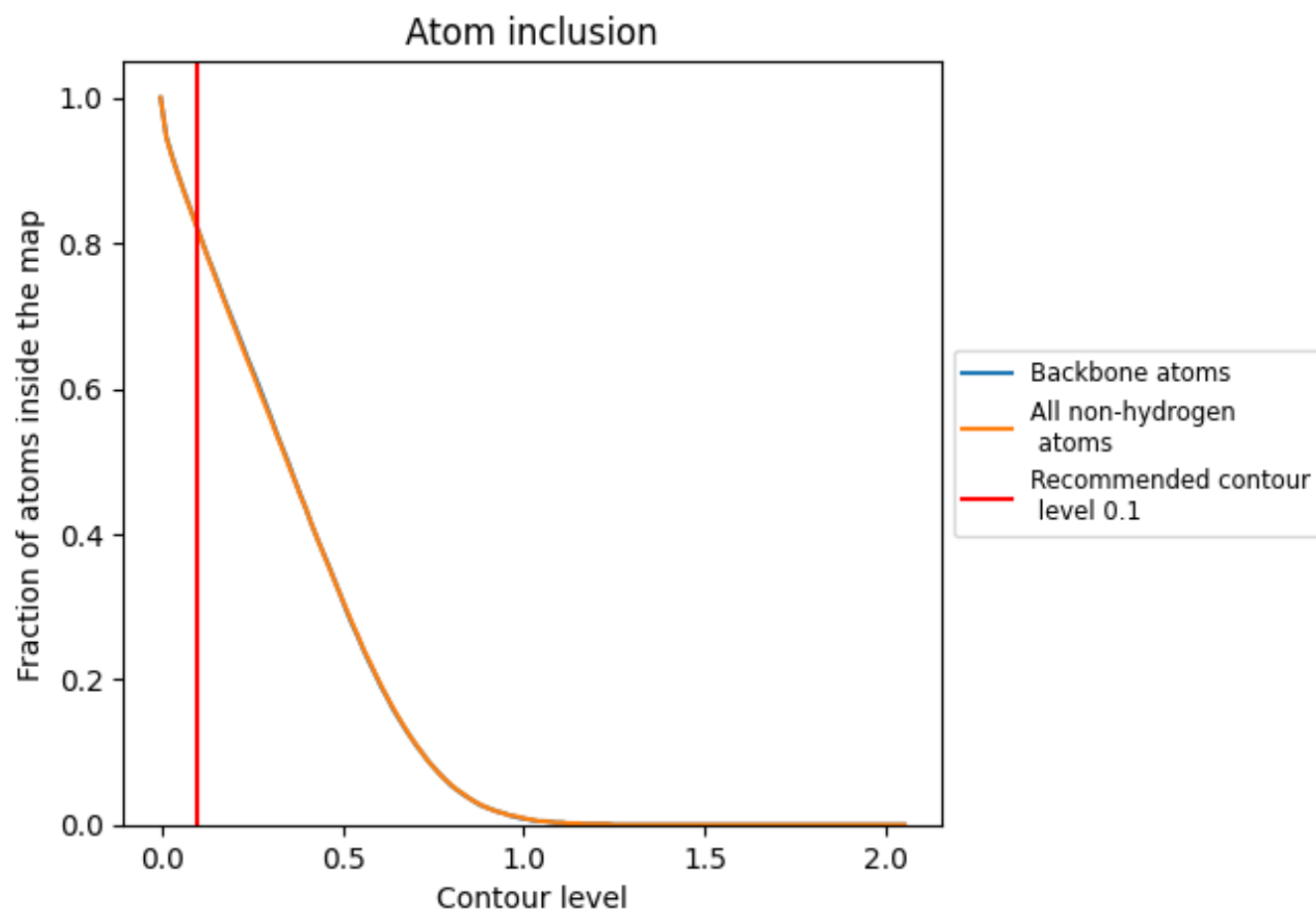
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.4730
Ja	 0.8070	 0.4930
Jb	 0.7650	 0.4720
Jc	 0.8190	 0.4910
Jd	 0.7610	 0.4580
Je	 0.8230	 0.5010
Jf	 0.7760	 0.4740
Ka	 0.8730	 0.5040
Kb	 0.8850	 0.5240
Kc	 0.8870	 0.5140
La	 0.8720	 0.5000
Lb	 0.8630	 0.4790
Lc	 0.8430	 0.4770
Ld	 0.8490	 0.4670
Le	 0.8740	 0.4870
Lf	 0.8350	 0.4490
Lg	 0.8270	 0.4640
Lh	 0.8810	 0.4930
Li	 0.8670	 0.4740
Ma	 0.8520	 0.5170
Mb	 0.8240	 0.4880
Mc	 0.8410	 0.4970
Md	 0.8180	 0.4950
Me	 0.8470	 0.5240
Mf	 0.8280	 0.5110
Na	 0.7840	 0.4720
Nb	 0.7780	 0.4760
Nc	 0.7890	 0.4740
Oa	 0.8880	 0.5440
Ob	 0.9000	 0.5570
Oc	 0.9000	 0.5580
Pa	 0.7930	 0.4150
Pb	 0.8030	 0.4280
Pc	 0.8040	 0.4260
Qa	 0.6200	 0.2700



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Chain	Atom inclusion	Q-score
Qb	 0.6210	 0.2750
Qc	 0.6270	 0.2880
Ra	 0.8050	 0.4040
Rb	 0.8000	 0.3860
Rc	 0.7940	 0.4120
Rd	 0.7640	 0.3150
Re	 0.7680	 0.3030
Rf	 0.7750	 0.3310
Sa	 0.8060	 0.4400
Sb	 0.8150	 0.4460
Sc	 0.8150	 0.4580