



## wwPDB EM Validation Summary Report ⓘ

Apr 19, 2025 – 12:40 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.dev117  
MolProbity : 4.02b-467  
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) : 2.42

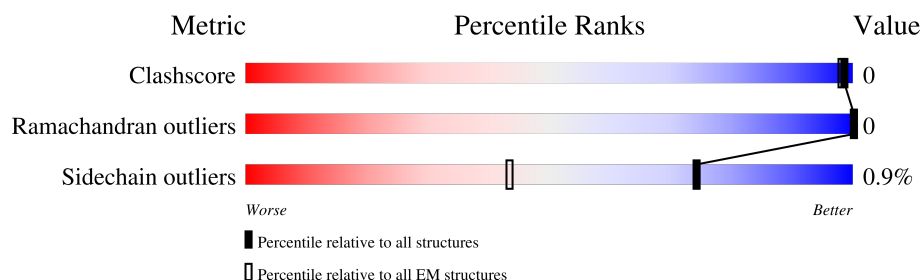
# 1 Overall quality at a glance

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.











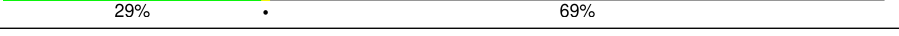

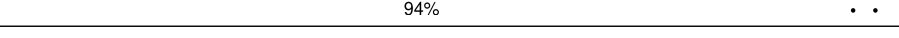
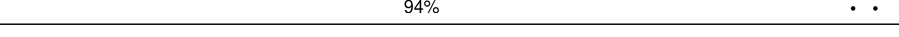
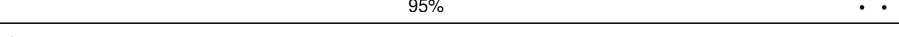
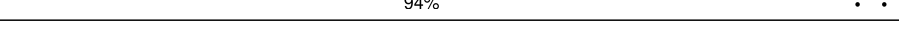
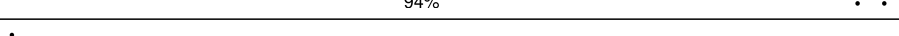
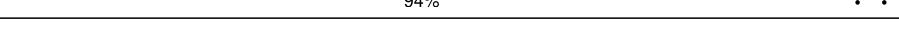
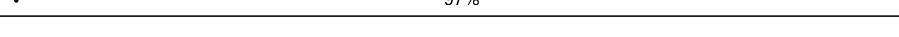
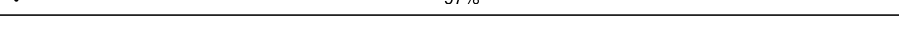
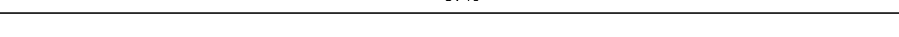






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 10% 97%
1	Jb	283	 10% 97%
1	Jc	283	 10% 98%
1	Jd	283	 10% 96%
1	Je	283	 10% 98%
1	Jf	283	 7% 96%
2	Ka	86	 93%
2	Kb	86	 93%

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

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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		

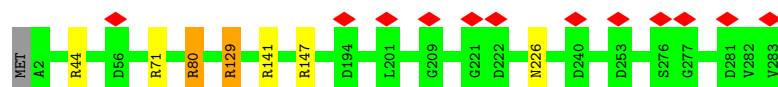


### 3 Residue-property plots [i](#)

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.

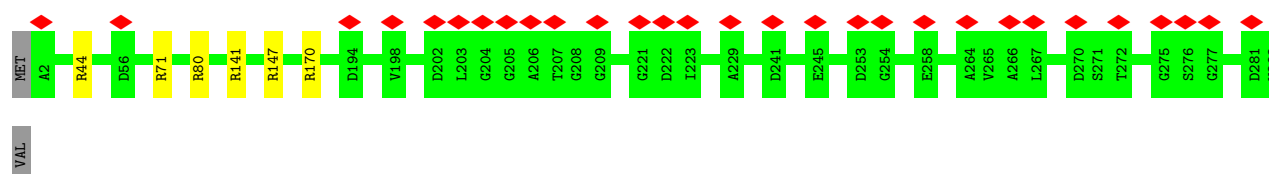
- Molecule 1: Tail tube, gp19

Chain Ja:  97%



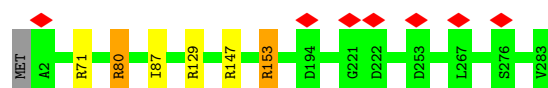
- Molecule 1: Tail tube, gp19

Chain Jb:  97%



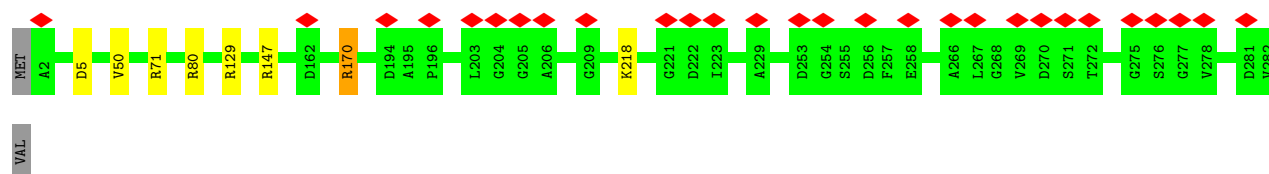
- Molecule 1: Tail tube, gp19

Chain Jc:  98%




- Molecule 1: Tail tube, gp19

Chain Jd:  96%



- Molecule 1: Tail tube, gp19

Category	Gene Count
MET	1
A2	1
R44	1
R80	1
R129	1
D139	1
R147	1
R153	1
L201	1
G221	1
D222	1
D253	1
G277	1
D281	1
V282	1
V283	1

- Chain Jf: 

- Chain Ka:  93%

- Chain Kb:  93% ...

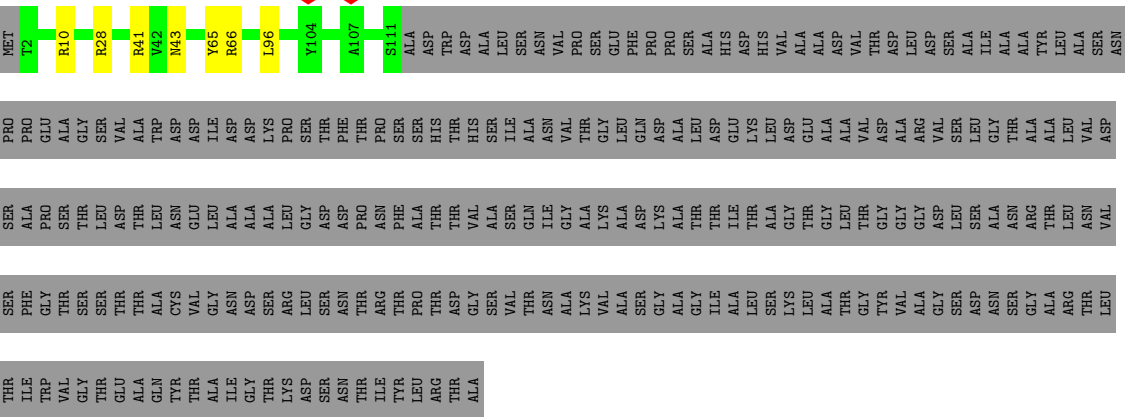
- Chain Kc:  91% 6%

- Chain La:  29% 69%

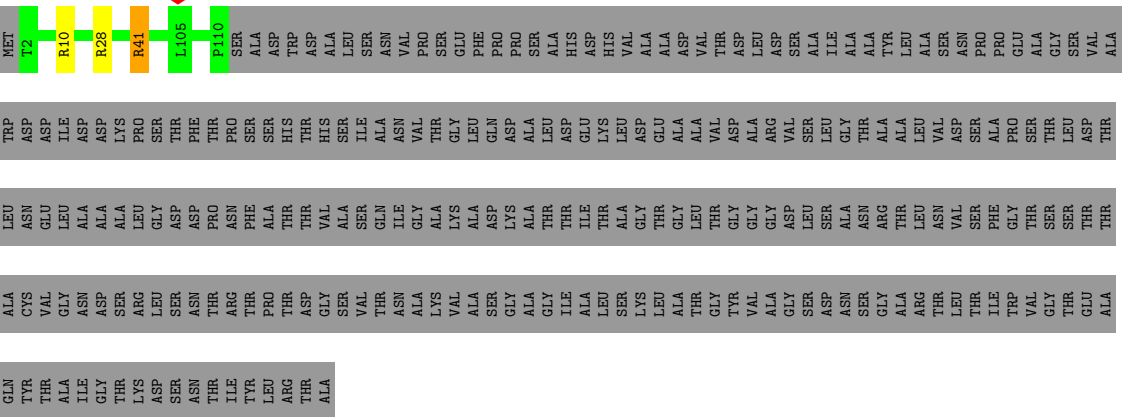
THR	ALA	THR	ALA
ALA	ASN	ASN	TRP
CYS	GLU	GLY	ASP
VAL	GLY	ALA	ILE
ASN	ALA	ASP	ASP
ASP	ASP	ASP	ASP
SER	ALA	LYS	LYS
ARG	LEU	PRO	PRO
LEU	GLY	SER	SER
ASP	ASP	THR	THR
ASN	ASP	PHE	PHE
THR	PRO	THR	THR
THR	THR	THR	THR
ASP	THR	THR	THR
GLY	VAL	THR	THR
SER	ALA	SER	ALA
VAL	SER	ILE	SER
THR	THR	GLN	ALA
ASN	ILE	ASN	VAL
ALA	GLY	VAL	PRO
VAL	LYS	ALA	SER
VAL	VAL	GLY	GLY
ALA	ALA	LEU	PHE
SER	SER	ASP	PRO
GLY	GLY	LYS	PRO
ALA	ALA	ALA	SER
ILE	THR	THR	ALA
ALA	ILE	GLU	HIS
LEU	THR	LYS	ASP
SER	ALA	LEU	HIS
LYS	GLY	ASP	VAL
LEU	THR	GLU	ALA
THR	GLY	ALA	ALA
THR	LEU	ALA	ASP
GLY	THR	VAL	VAL
THR	GLY	ASP	THR
VAL	GLY	ALA	ASP
GLY	GLY	ALA	LEU
GLY	GLY	ARG	ASP
SER	ASP	VAL	SER
SER	LEU	SER	ALA
ASP	SER	LEU	ILE
ASN	ALA	GLY	ALA
SER	ASN	THR	ALA
GLY	ARG	ALA	THR
ALA	THR	ALA	TRP
ARG	LEU	LEU	LEU
THR	ASN	VAL	ALA
LEU	VAL	ASP	SER
THR	SER	SER	ASN
ILE	PHE	THR	PRO
TRP	GLY	ALA	GLU
VAL	VAL	SER	PRO
GLY	THR	SER	ALA
THR	SER	LEU	GLY
			SER

ALA  
GLN  
TYR  
THR  
ALA  
ILE  
GLY  
THR  
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SER  
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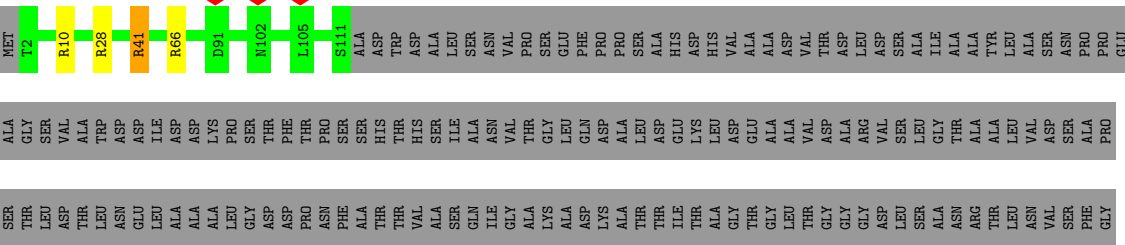
• Molecule 3: Tail collar fibers, gp4



• Molecule 3: Tail collar fibers, gp4



• Molecule 3: Tail collar fibers, gp4



[illegible]

- Molecule 3: Tail collar fibers, gp4

Chain Le:  29% 69%

ALA	GLN	ALA	THR	THR	LEU	THR	ALA	TRP	MET
TYR	THR	CYS	ALA	ASN	ASP	ASN	TRP	T2	
ALA	ALA	VAL	VAL	GLU	LEU	GLU	ASP	R10	
ILE	ILE	GLY	GLY	LEU	ALA	ILE	ILE	R41	
GLY	ASP	ASN	ASP	ALA	ALA	ASP	ASP		
THR	SER	SER	SER	ALA	ALA	LYS	LYS	Y65	
LYS	ASP	LEU	GLY	LEU	LEU	PRO	PRO	R66	
ASP	SER	ASP	ASP	GLY	GLY	SER	SER		
SER	SER	ASN	ASN	ASP	ASP	PHE	PHE	L97	
THR	THR	THR	THR	PRO	PRO	THR	THR		
ILE	ARG	ARG	THR	ASN	ASN	PRO	PRO	P110	
TYR	TYR	THR	THR	PHE	SER	SER	SER	SER	
LEU	LEU	ALA	ALA	ALA	SER	HIS	ASP	ALA	
ARG	ARG	THR	THR	THR	THR	HIS	THR	THR	
THR	THR	ASP	GLY	VAL	VAL	HIS	THR	ASP	
ALA	ALA			ALA	ALA	HIS	HIS	ALA	
				SER	SER	SER	SER	LEU	
				VAL	LYS	GLY	GLY	LEU	
				VAL	ALA	ALA	ILE	LEU	
				ASN	GLN	ASN	ASN	ASN	
				ILE	ILE	VAL	VAL	PRO	
				LYS	ALA	THR	THR	SER	
				VAL	LYS	GLY	GLY	SER	
				VAL	ALA	ALA	LEU	PHE	
				THR	THR	THR	THR	PRO	
				ILE	ILE	GLU	LYS	ASP	
				LEU	THR	THR	HIS	PRO	
				SER	ALA	LEU	HIS	SER	
				LYS	GLY	ASP	VAL	ALA	
				LEU	THR	THR	ALA	ALA	
				THR	THR	GLY	GLY	ASP	
				ALA	GLY	GLU	ASP	LEU	
				THR	LEU	ALA	VAL	ASP	
				GLY	THR	VAL	THR	SER	
				TVR	GLY	ASP	ASP	THR	
				VAL	GLY	ALA	ALA	LEU	
				ALA	GLY	ARG	ARG	ASP	
				GLY	ASP	VAL	VAL	SER	
				SER	SER	LEU	ILE	ALA	
				ASN	ALA	GLY	GLY	ALA	
				SER	ARG	THR	THR	ALA	
				ALA	ARG	LEU	ALA	LEU	
				THR	THR	ASN	VAL	SER	
				LEU	VAL	ASP	ASP	ASN	
				THR	SER	SER	SER	PRO	
				ILE	PHE	GLY	ALA	PRO	
				THR	THR	THR	PRO	GLU	
				VAL	SER	SER	SER	ALA	
				GLY	THR	THR	THR	GLY	
				THR	THR	THR	THR	SER	
				GLN	THR	THR	LEU	VAL	

- Molecule 3: Tail collar fibers, gp4

Chain Lf:  29% .. 69%

Ile	Phe	Pro	Met
Trp	Gly	Glu	T2
Val	Thr	Ala	
Gly	Ser	Gly	V9
Thr	Ser	Ser	R10
Glu	Thr	Val	
Ala	Thr	Ala	R28
Gln	Ala	Trp	Q29
Thr	Cys	Asp	
Val	Val	Asp	R41
Ala	Gly	Ile	
Ala	Asn	Asp	R66
Gly	Asp	Asp	
Thr	Ser	Lys	D91
Lys	Arg	Pro	
Asp	Leu	Ser	E95
Ser	Ser	Thr	L96
Asn	Asn	Phe	
Thr	Thr	Thr	
Ile	Arg	Pro	P110
Tyr	Thr	Ser	Ser
Leu	Pro	Ser	Ala
Arg	Thr	His	ASP
Thr	Asp	Thr	TRP
Ala	Gly	HIS	ASP
	Ser	SER	ALA
	Val	ILE	LEU
	Thr	ALA	SER
	Asn	ASN	VAL
	Ala	VAL	VAL
	Lys	THR	PRO
	Val	GLY	SER
	Ala	LEU	GLU
	Ser	GLN	PHE
	Gly	ASP	PRO
	Ala	ALA	SER
	Gly	LEU	ALA
	Ile	THR	HIS
	Ala	GLU	ASP
	Leu	LYS	HIS
	Ser	LEU	ASP
	Lys	ASP	VAL
	Leu	GLU	ALA
	Ala	ALA	ASP
	Thr	VAL	VAL
	Gly	THR	THR
	Tyr	ASP	ASP
	Ala	ALA	LEU
	Gly	ARG	ASP
	Ser	VAL	SER
	Gly	SER	ALA
	Asp	LEU	ILE
	Asn	ALA	ALA
	Ser	THR	ALA
	Gly	ARG	TYR
	Ala	THR	LEU
	Arg	ASN	ALA
	Thr	VAL	SER
	Leu	SER	ASN

- Molecule 3: Tail collar fibers, gp4

Chain Lg:  30% 69%

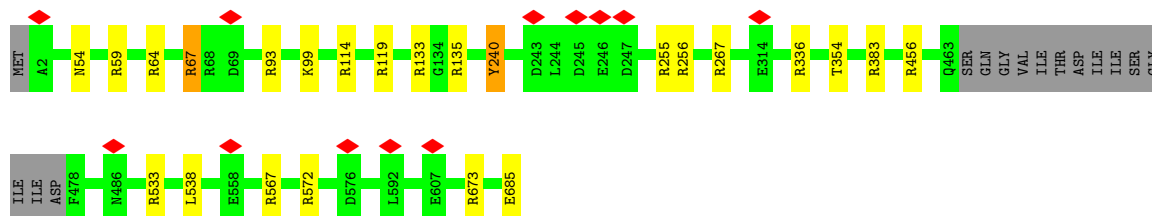
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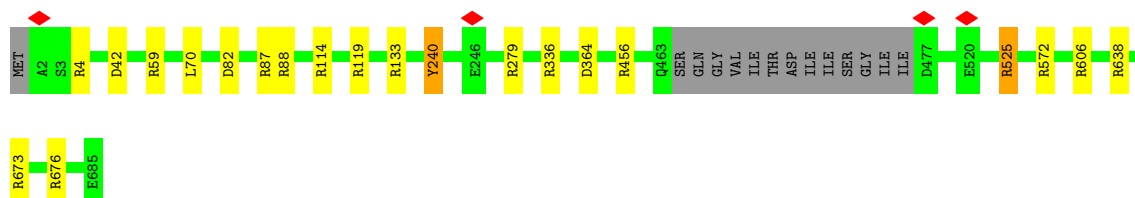
- Molecule 4: Tail tip cage, gp23

Chain Mb: 94%



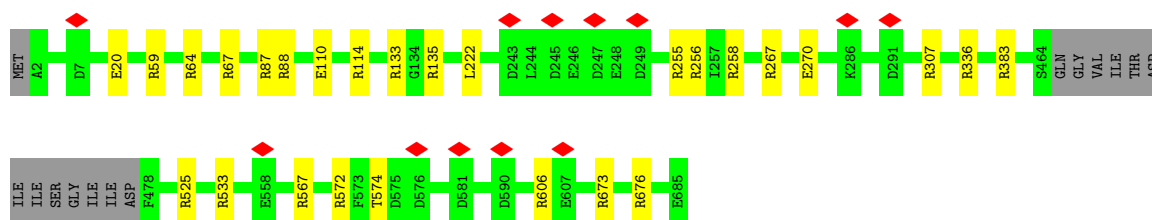
- Molecule 4: Tail tip cage, gp23

Chain Mc: 95%



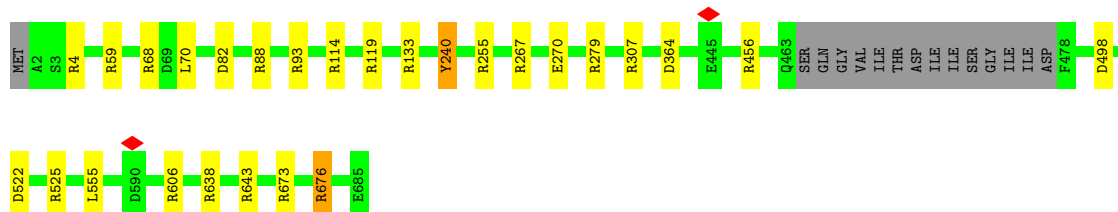
- Molecule 4: Tail tip cage, gp23

Chain Md: 94%

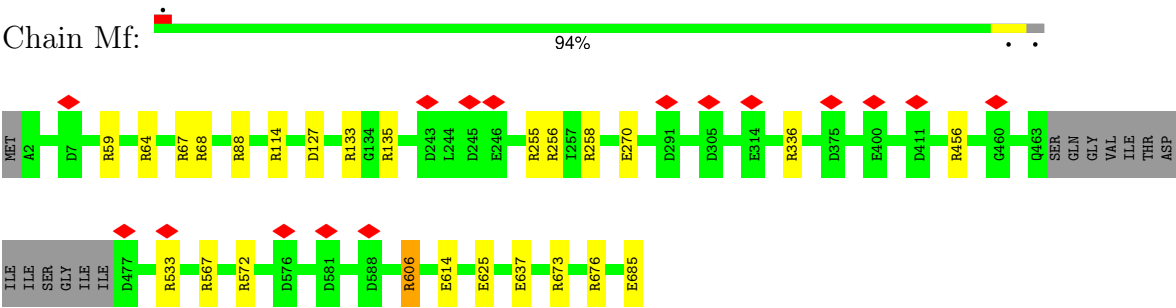


- Molecule 4: Tail tip cage, gp23

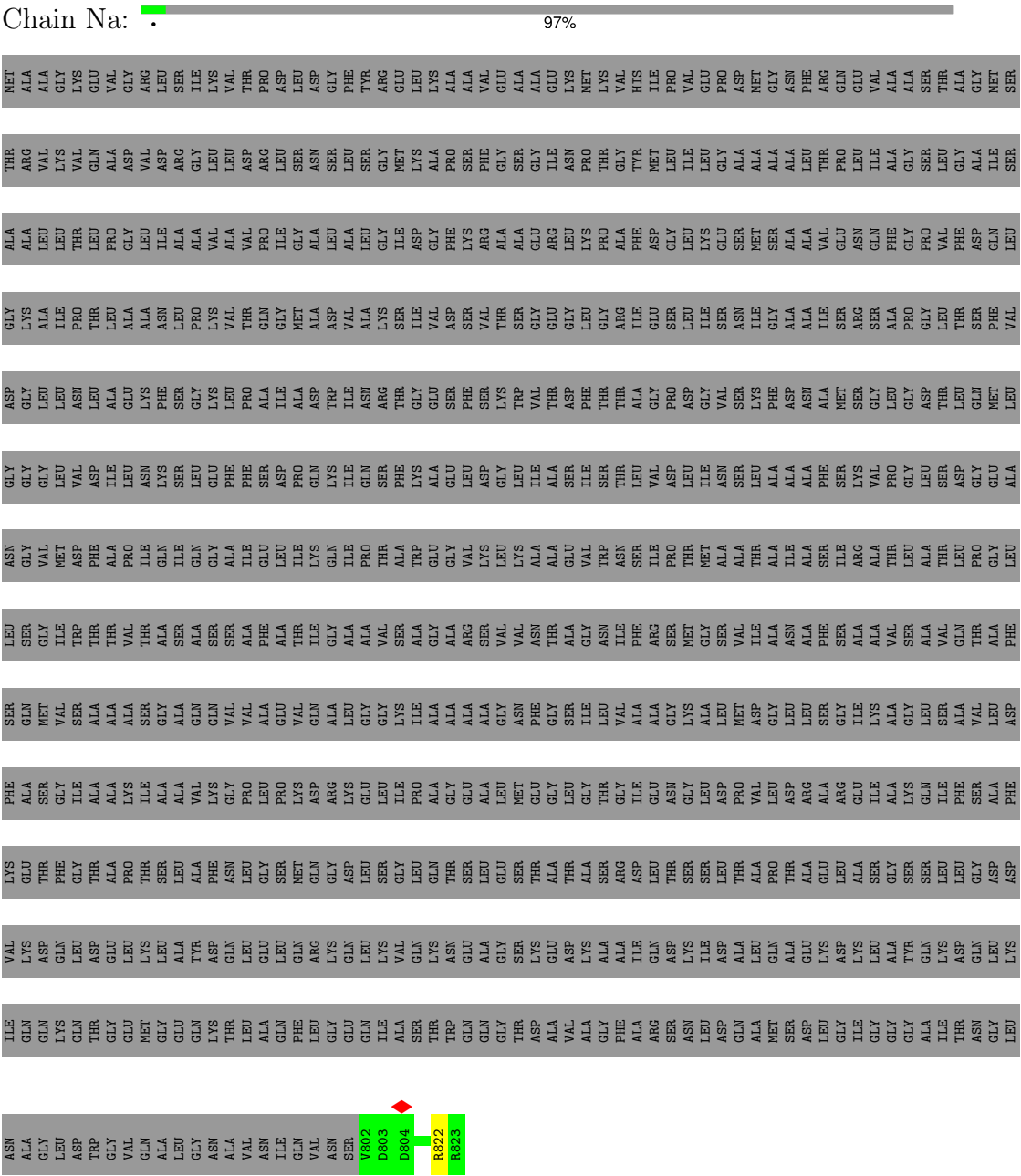
Chain Me: 94%



- Molecule 4: Tail tip cage, gp23



● Molecule 5: Tapemeasure protein



● Molecule 5: Tapemeasure protein

97%

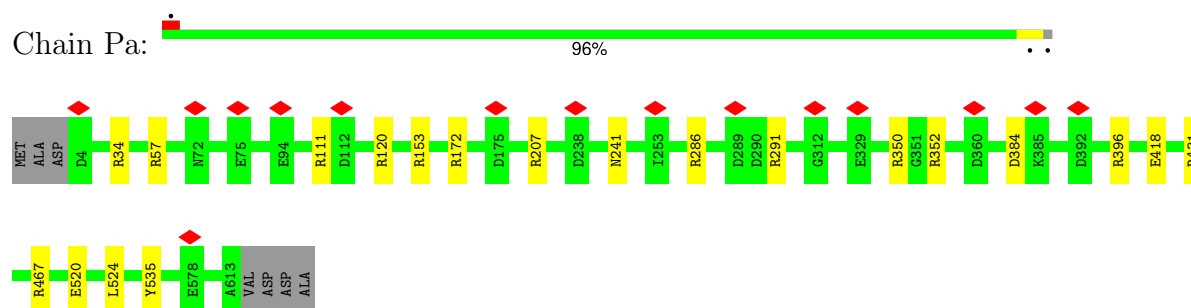
A diagram showing a red diamond symbol above a green box containing 'V802' and 'D803', which is connected to an orange box containing 'R823'.

## 97%

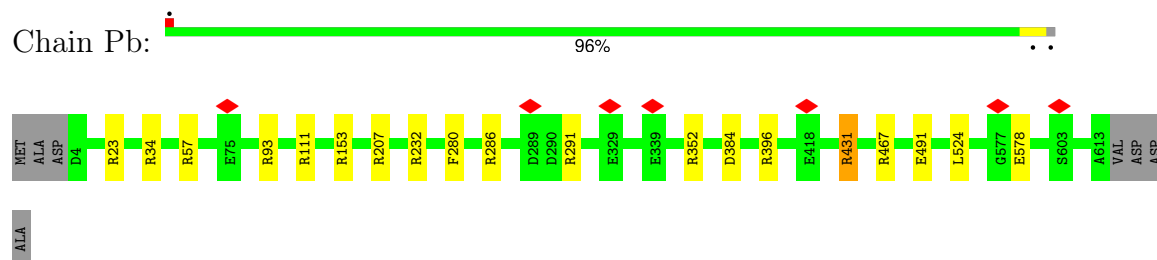
GLY  
LYS  
ALA  
ILE  
PRO  
THR  
LEU  
ALA  
ASN  
LEU  
PRO  
LYS  
VAL  
THR  
GLN  
GLY  
MET  
ALA  
ASP  
VAL  
ALA  
LYS  
SER  
LEU  
VAL  
THR  
SER  
GLY  
GLU  
GLY  
LEU  
GLY  
ARG  
ILE  
GLU  
SER  
SER  
ILE  
SER  
ASN  
ILE  
GLY  
ALA  
ALA  
SER  
ARG  
SER  
ALA  
PRO  
GLY  
LEU  
THR  
SER  
PHE



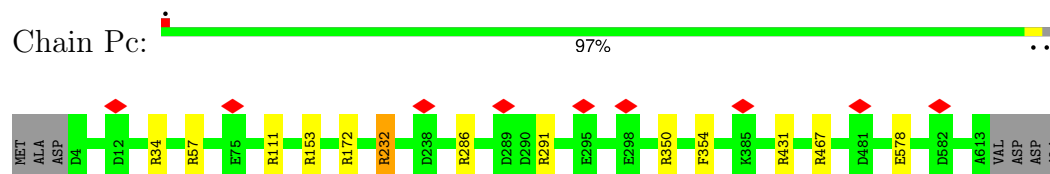
- Molecule 7: Tail spike, gp29



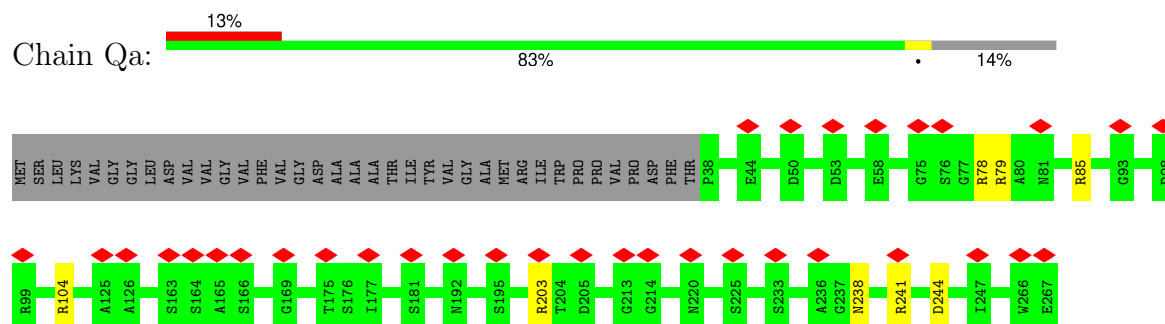
- Molecule 7: Tail spike, gp29



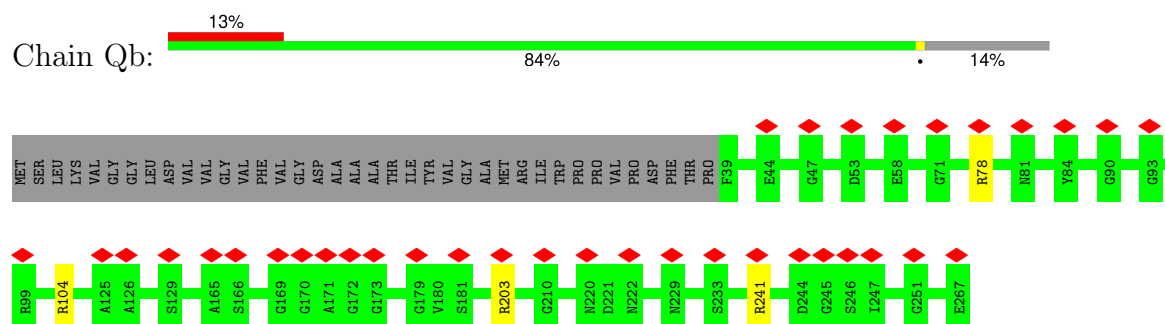
- Molecule 7: Tail spike, gp29



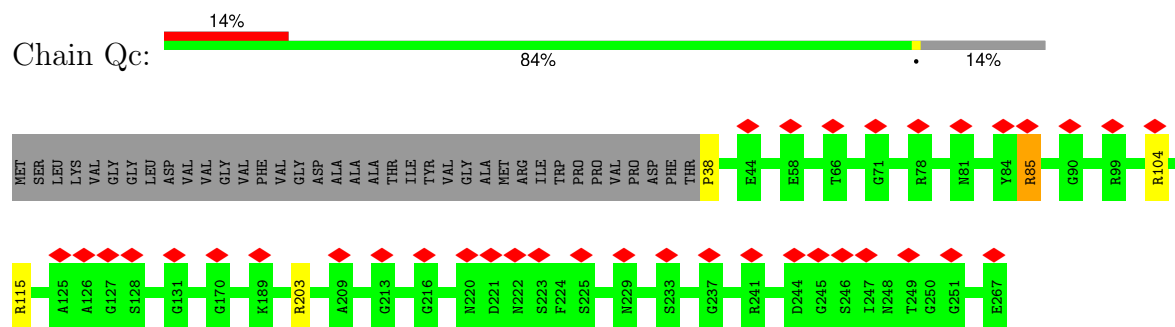
- Molecule 8: Tail wing brush, gp33



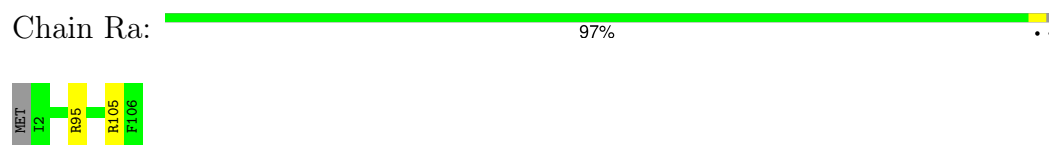
- Molecule 8: Tail wing brush, gp33



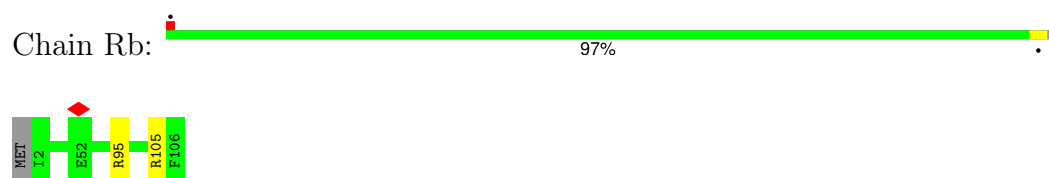
- Molecule 8: Tail wing brush, gp33



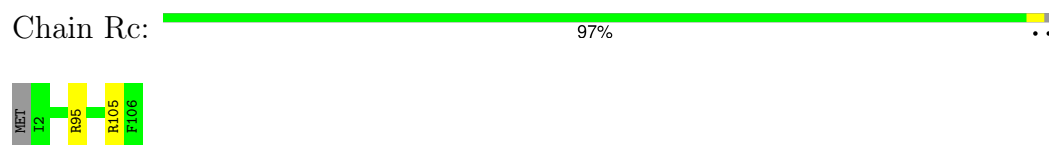
- Molecule 9: Tail wing arm, gp31



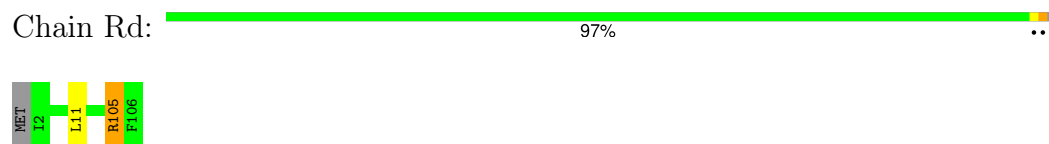
- Molecule 9: Tail wing arm, gp31



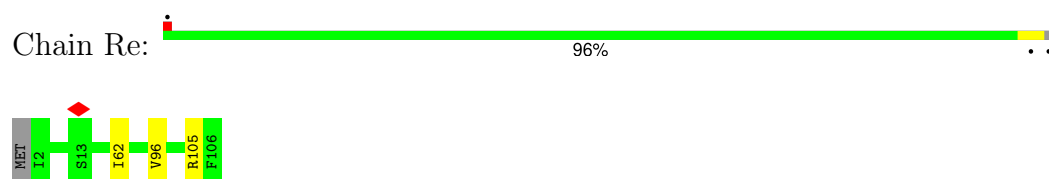
- Molecule 9: Tail wing arm, gp31



- Molecule 9: Tail wing arm, gp31



- Molecule 9: Tail wing arm, gp31



- Molecule 9: Tail wing arm, gp31

- Chain Sa:  93%

[illegible]

- Chain Sb:  93%

- Chain Sc: 

## 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 ( $\text{\AA}$ )	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	0.61	0/2167	1.00	6/2958 (0.2%)
1	Jb	0.62	0/2159	0.99	6/2948 (0.2%)
1	Jc	0.61	0/2167	0.99	5/2958 (0.2%)
1	Jd	0.62	0/2159	1.00	6/2948 (0.2%)
1	Je	0.61	0/2167	1.00	4/2958 (0.1%)
1	Jf	0.62	0/2167	0.99	6/2958 (0.2%)
2	Ka	0.61	0/678	1.05	3/932 (0.3%)
2	Kb	0.60	0/678	1.07	3/932 (0.3%)
2	Kc	0.60	0/678	1.08	4/932 (0.4%)
3	La	0.59	0/852	0.99	3/1174 (0.3%)
3	Lb	0.61	0/858	1.02	4/1182 (0.3%)
3	Lc	0.61	0/852	1.02	3/1174 (0.3%)
3	Ld	0.62	0/858	1.03	4/1182 (0.3%)
3	Le	0.59	0/852	0.98	3/1174 (0.3%)
3	Lf	0.60	0/852	0.99	4/1174 (0.3%)
3	Lg	0.60	0/852	0.96	1/1174 (0.1%)
3	Lh	0.61	0/858	1.05	4/1182 (0.3%)
3	Li	0.62	0/858	1.05	4/1182 (0.3%)
4	Ma	0.64	0/5265	1.04	16/7203 (0.2%)
4	Mb	0.64	0/5265	1.01	18/7203 (0.2%)
4	Mc	0.64	0/5273	1.03	16/7214 (0.2%)
4	Md	0.64	0/5271	1.02	21/7211 (0.3%)
4	Me	0.64	0/5265	1.02	19/7203 (0.3%)
4	Mf	0.64	0/5273	1.03	20/7214 (0.3%)
5	Na	0.65	0/176	1.07	0/237
5	Nb	0.63	0/176	1.08	1/237 (0.4%)
5	Nc	0.62	0/176	1.07	1/237 (0.4%)
6	Oa	0.64	0/4844	1.03	18/6597 (0.3%)
6	Ob	0.64	0/4844	1.05	18/6597 (0.3%)
6	Oc	0.64	0/4844	1.03	16/6597 (0.2%)
7	Pa	0.59	0/4563	0.99	16/6227 (0.3%)
7	Pb	0.59	0/4563	0.99	12/6227 (0.2%)
7	Pc	0.58	0/4563	0.97	13/6227 (0.2%)
8	Qa	0.66	0/1494	0.94	6/2006 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	Qb	0.65	0/1486	0.91	4/1995 (0.2%)
8	Qc	0.64	0/1494	0.94	5/2006 (0.2%)
9	Ra	0.60	0/811	0.93	2/1114 (0.2%)
9	Rb	0.60	0/811	0.95	2/1114 (0.2%)
9	Rc	0.60	0/811	0.92	2/1114 (0.2%)
9	Rd	0.64	0/811	1.01	1/1114 (0.1%)
9	Re	0.62	0/811	1.00	1/1114 (0.1%)
9	Rf	0.63	0/811	0.97	1/1114 (0.1%)
10	Sa	0.63	0/3831	1.01	9/5228 (0.2%)
10	Sb	0.64	0/3816	1.03	16/5207 (0.3%)
10	Sc	0.64	0/3816	1.02	9/5207 (0.2%)
All	All	0.63	0/103876	1.01	336/141886 (0.2%)

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 336 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Mf	133	ARG	NE-CZ-NH2	10.18	125.39	120.30
6	Ob	55	ARG	NE-CZ-NH2	10.01	125.31	120.30
4	Me	133	ARG	NE-CZ-NH2	9.93	125.27	120.30
1	Jc	129	ARG	NE-CZ-NH2	9.69	125.14	120.30
6	Ob	311	ARG	NE-CZ-NH2	9.55	125.07	120.30

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	0	0
1	Jc	2124	2039	2038	0	0
1	Jd	2116	2030	2029	0	0
1	Je	2124	2039	2038	0	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	0	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	0	0
4	Ma	5141	4965	4963	0	0
4	Mb	5141	4965	4963	0	0
4	Mc	5149	4969	4967	0	0
4	Md	5147	4970	4968	0	0
4	Me	5141	4963	4963	0	0
4	Mf	5149	4968	4967	0	0
5	Na	176	179	178	0	0
5	Nb	176	179	178	0	0
5	Nc	176	179	178	0	0
6	Oa	4705	4604	4602	0	0
6	Ob	4705	4603	4602	0	0
6	Oc	4705	4603	4602	0	0
7	Pa	4466	4361	4359	0	0
7	Pb	4466	4360	4359	0	0
7	Pc	4466	4360	4359	0	0
8	Qa	1472	1336	1336	0	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	0	0
10	Sb	3714	3532	3531	0	0
10	Sc	3714	3532	3531	0	0
All	All	101450	97837	97789	0	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.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	217 (99%)	3 (1%)	62	82
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%)	90 (99%)	1 (1%)	70	85
3	Lb	92/278 (33%)	90 (98%)	2 (2%)	47	71
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%)	88 (97%)	3 (3%)	33	59
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%)	90 (98%)	2 (2%)	47	71
4	Ma	555/568 (98%)	549 (99%)	6 (1%)	70	85
4	Mb	555/568 (98%)	550 (99%)	5 (1%)	75	88
4	Mc	556/568 (98%)	552 (99%)	4 (1%)	81	91
4	Md	556/568 (98%)	550 (99%)	6 (1%)	70	85
4	Me	555/568 (98%)	547 (99%)	8 (1%)	62	82
4	Mf	556/568 (98%)	548 (99%)	8 (1%)	62	82
5	Na	19/613 (3%)	18 (95%)	1 (5%)	19	38
5	Nb	19/613 (3%)	18 (95%)	1 (5%)	19	38
5	Nc	19/613 (3%)	18 (95%)	1 (5%)	19	38
6	Oa	496/500 (99%)	493 (99%)	3 (1%)	84	92
6	Ob	496/500 (99%)	492 (99%)	4 (1%)	79	90
6	Oc	496/500 (99%)	491 (99%)	5 (1%)	73	87
7	Pa	464/469 (99%)	459 (99%)	5 (1%)	70	85
7	Pb	464/469 (99%)	458 (99%)	6 (1%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Pc	464/469 (99%)	461 (99%)	3 (1%)	84	92
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%)	136 (99%)	1 (1%)	81	91
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%)	88 (99%)	1 (1%)	70	85
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%)	386 (99%)	5 (1%)	65	83
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%)	10649 (99%)	100 (1%)	74	88

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Na	822	ARG
6	Oc	430	MET
10	Sc	285	GLN
5	Nc	822	ARG
6	Ob	205	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	Jc	97	GLN
6	Ob	95	HIS

### 5.3.3 RNA ⓘ

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.

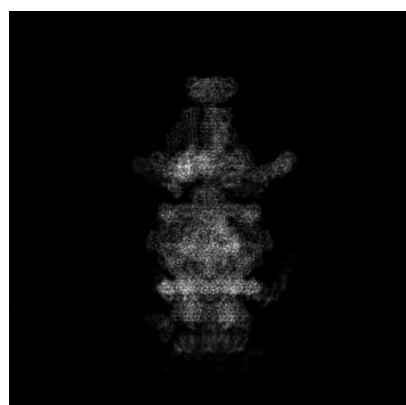
## 6 Map visualisation [i](#)

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.

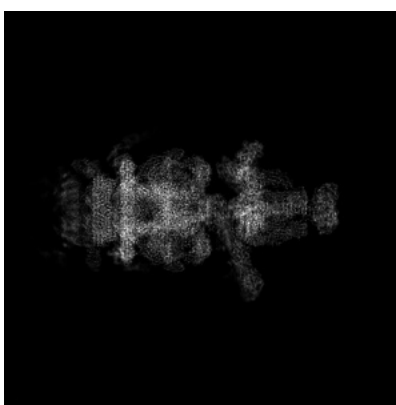
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

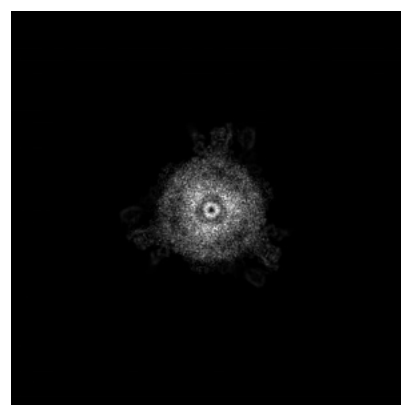
#### 6.1.1 Primary map



X



Y



Z

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

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

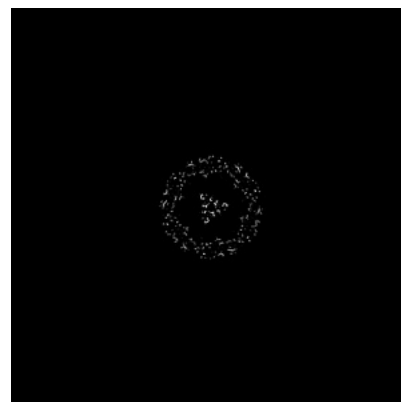
#### 6.2.1 Primary map



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](#)

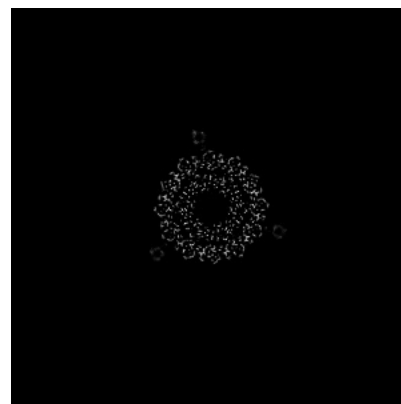
### 6.3.1 Primary map



X Index: 236



Y Index: 246

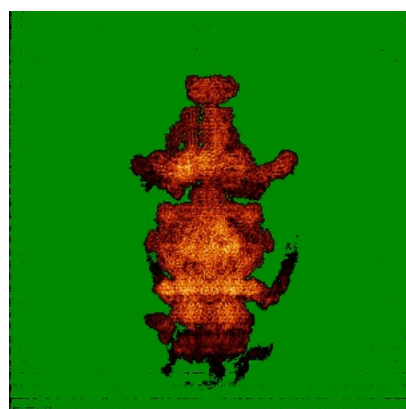


Z Index: 147

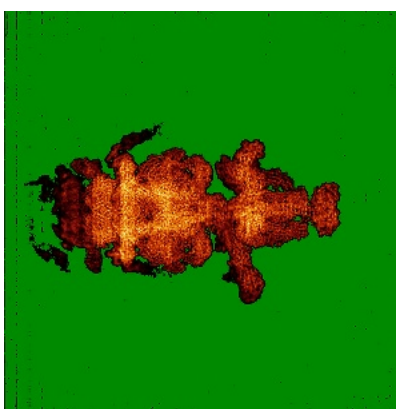
The images above show the largest variance slices of the map in three orthogonal directions.

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

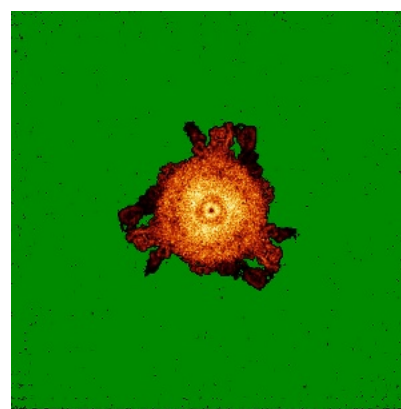
### 6.4.1 Primary map



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.

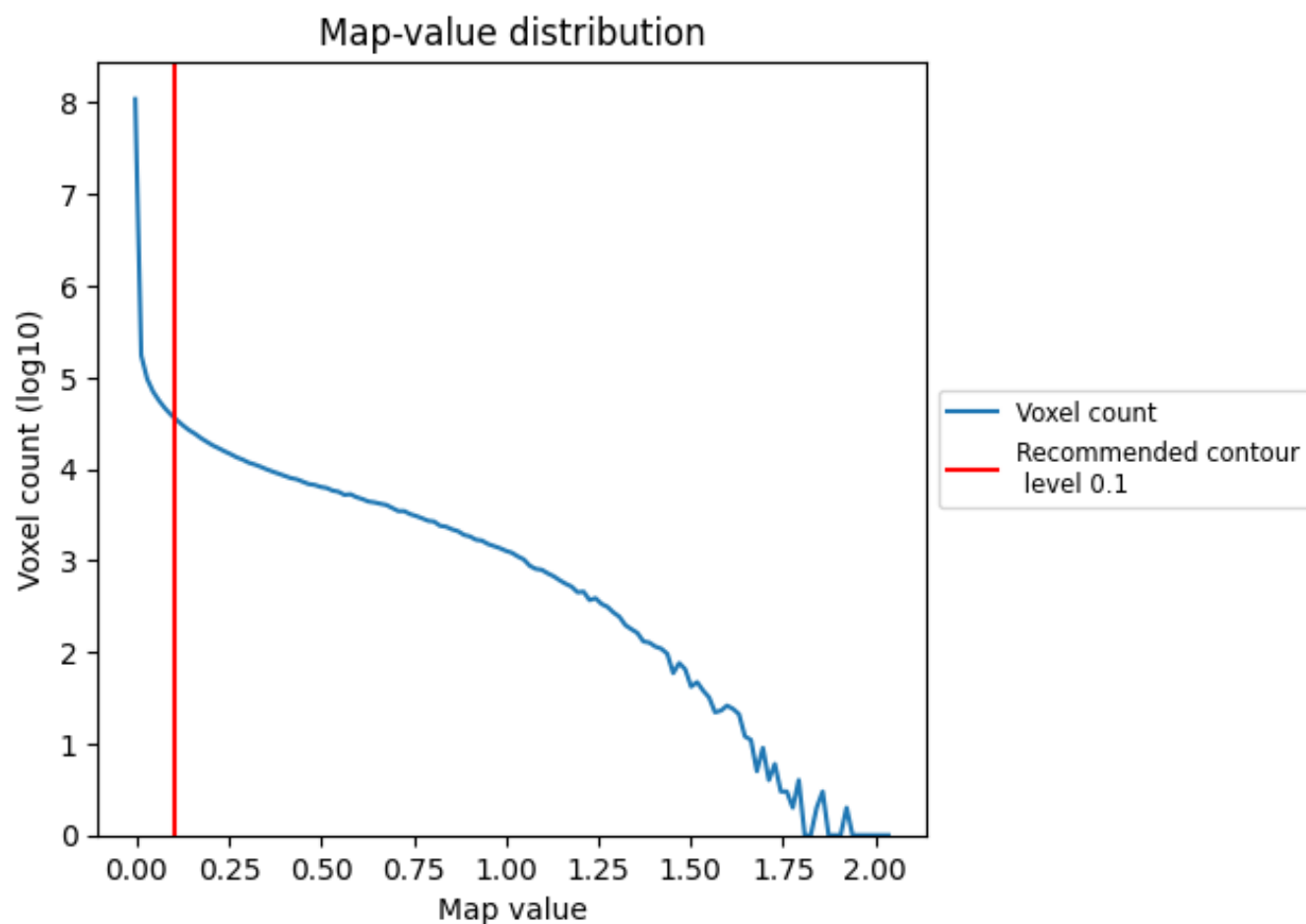
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

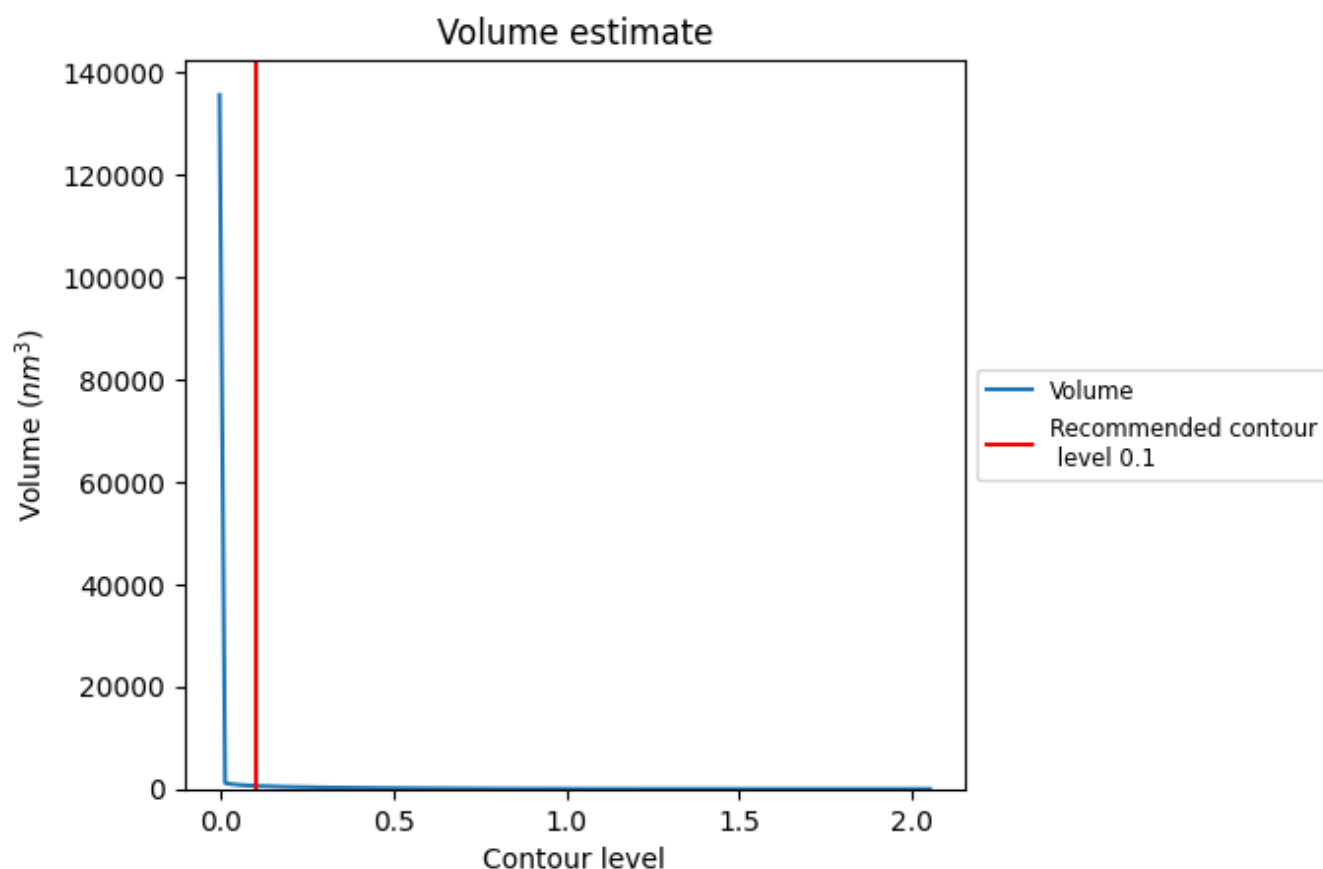
This section contains the results of statistical analysis of the map.

### 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.

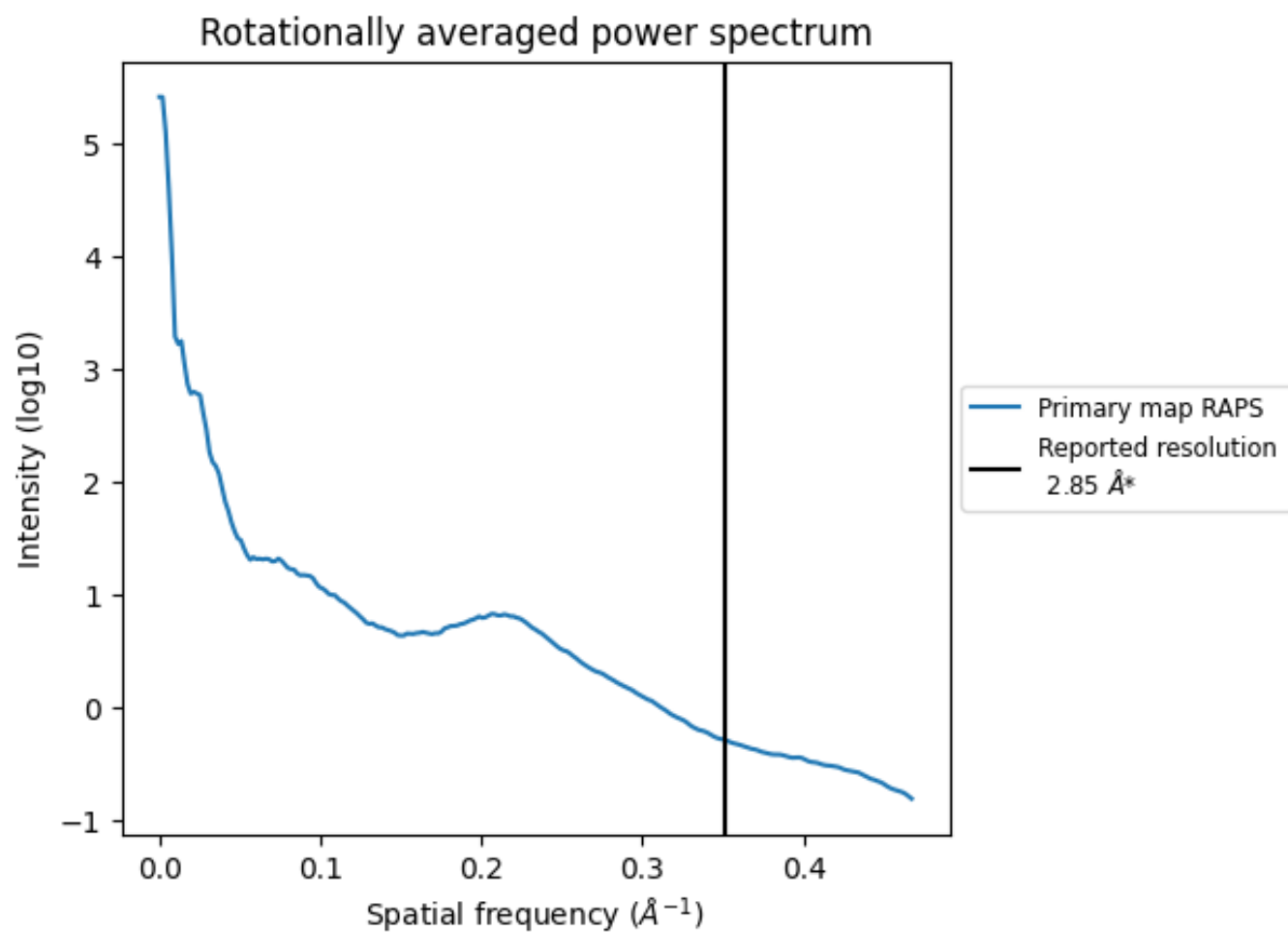
## 7.2 Volume estimate [i](#)



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>

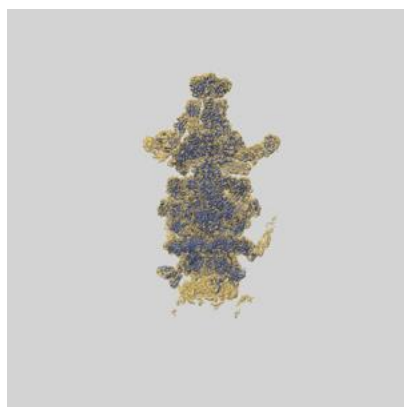
## 8 Fourier-Shell correlation

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

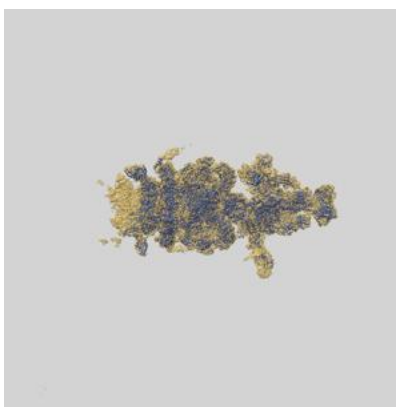
## 9 Map-model fit [i](#)

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](#).

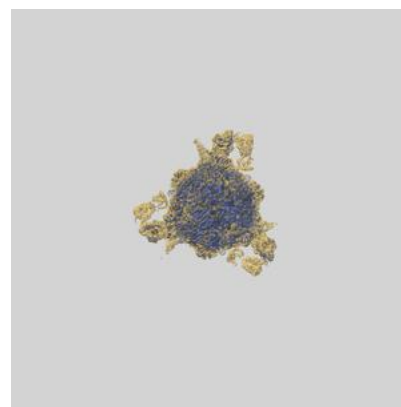
### 9.1 Map-model overlay [i](#)



X



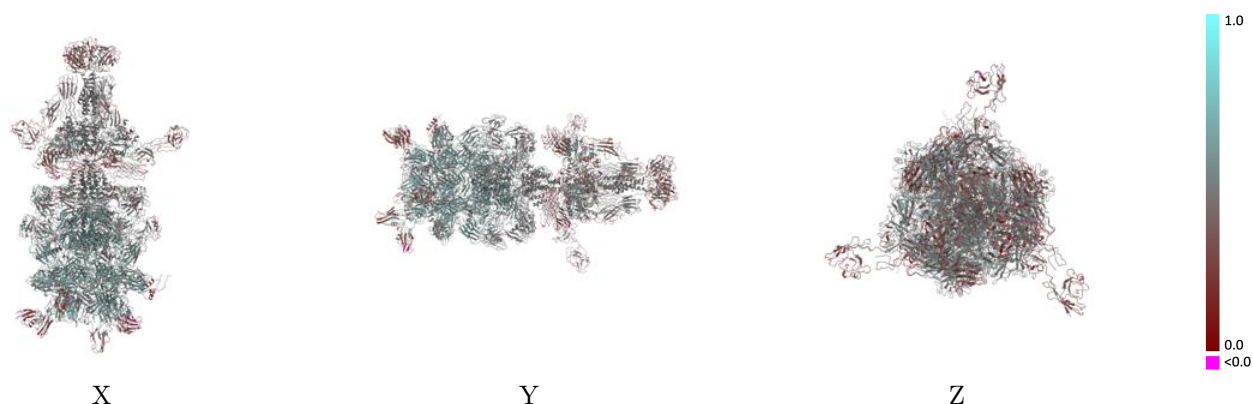
Y



Z

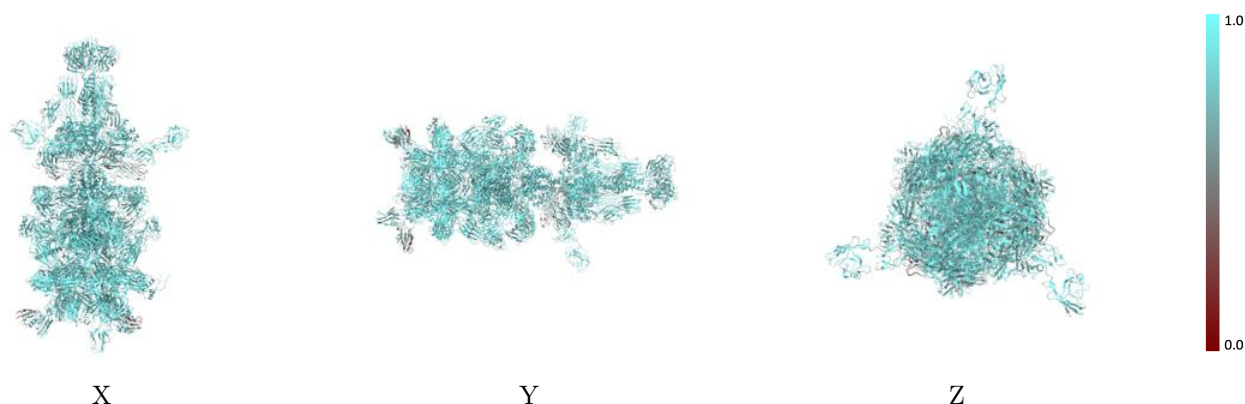
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



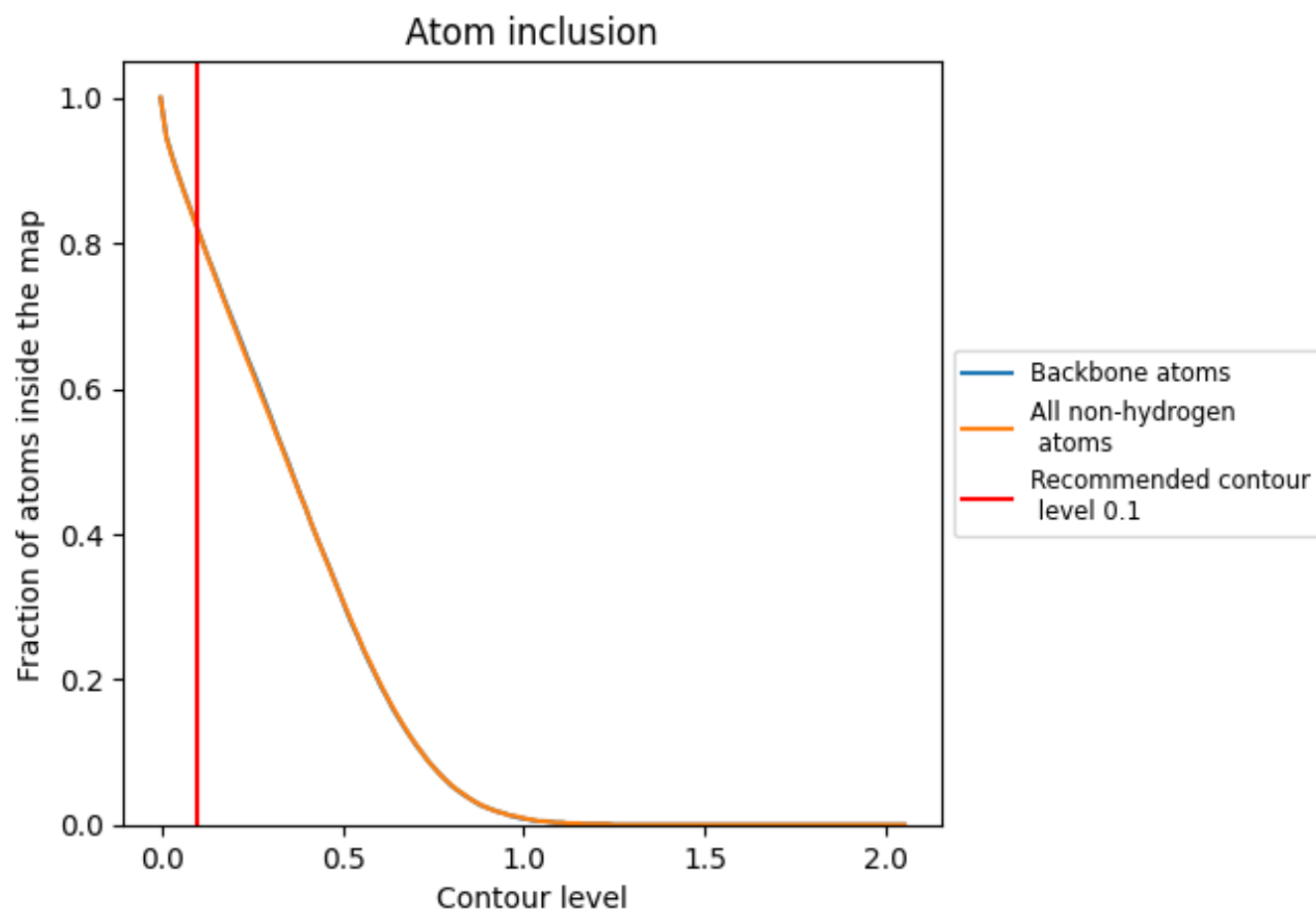
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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









































































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



*Continued on next page...*

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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