



Full wwPDB EM Validation Report ⓘ

May 31, 2025 – 01:07 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 Full wwPDB EM Validation 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.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

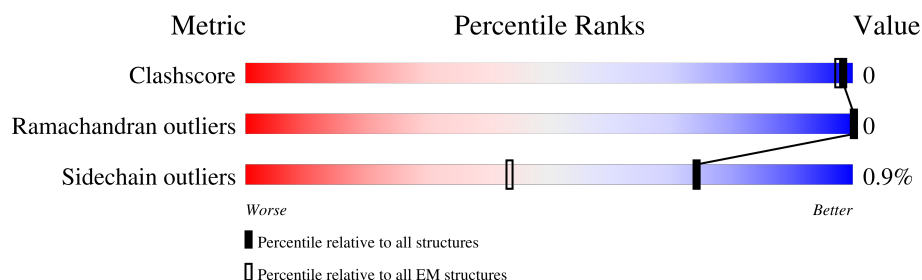
1 Overall quality at a glance

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.



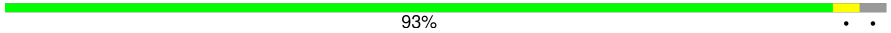














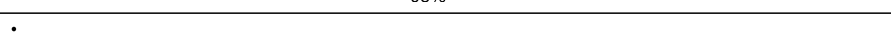
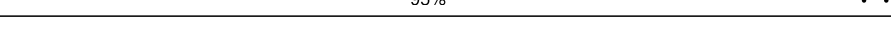
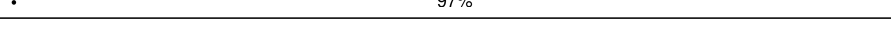
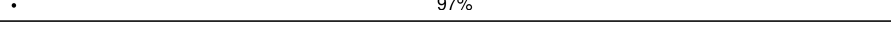
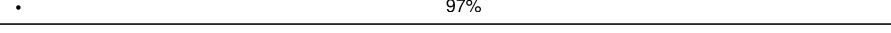
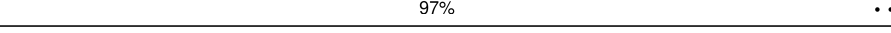
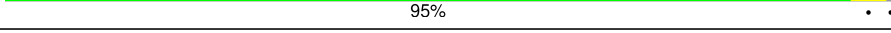
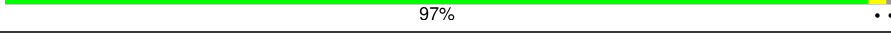
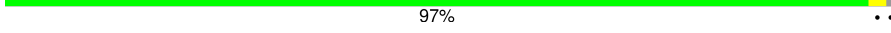
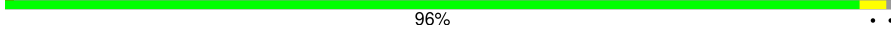
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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% 98% ..
1	Jb	283	 10% 98% ..
1	Jc	283	 10% 96% ..
1	Jd	283	 10% 96% ..
1	Je	283	 10% 98% .
1	Jf	283	 7% 97% .
2	Ka	86	 97% .
2	Kb	86	 95% ..




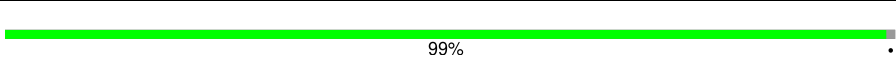
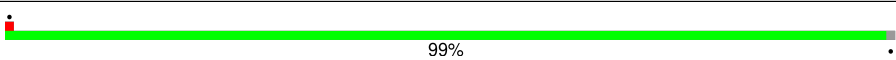
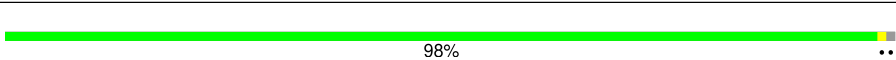
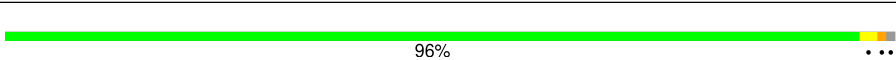
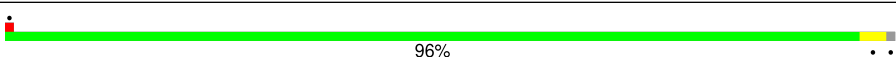
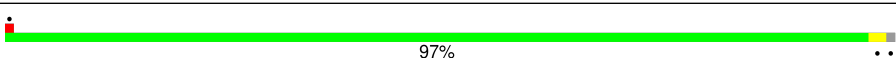
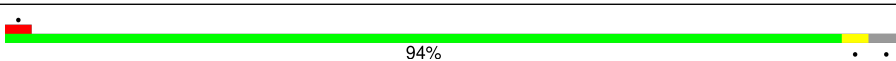
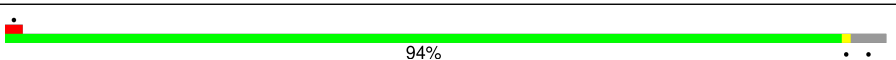
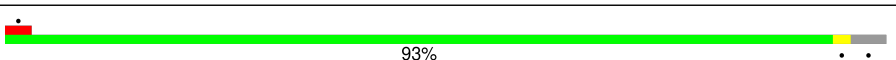
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Mol	Chain	Length	Quality of chain
2	Kc	86	 93%
3	La	356	 29% 69%
3	Lb	356	 29% 69%
3	Lc	356	 30% 69%
3	Ld	356	 30% 69%
3	Le	356	 29% 69%
3	Lf	356	 29% 69%
3	Lg	356	 30% 69%
3	Lh	356	 30% 69%
3	Li	356	 30% 69%
4	Ma	685	 94%
4	Mb	685	 95%
4	Mc	685	 95%
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.

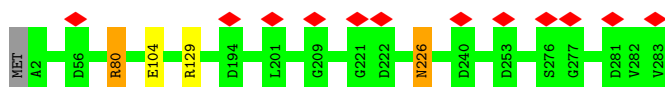
Mol	Chain	Residues	Atoms						AltConf	Trace
10	Sa	477	Total	C	H	N	O	S	0	0
			7279	2375	3550	613	725	16		
10	Sb	475	Total	C	H	N	O	S	0	0
			7246	2365	3532	611	722	16		
10	Sc	475	Total	C	H	N	O	S	0	0
			7246	2365	3532	611	722	16		

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.

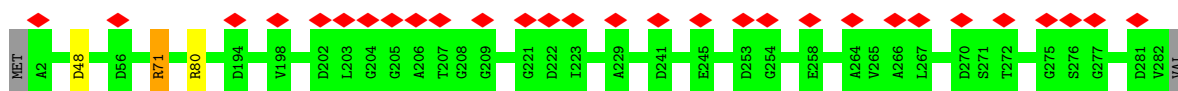
- Molecule 1: Tail tube, gp19

Chain Ja:  98%



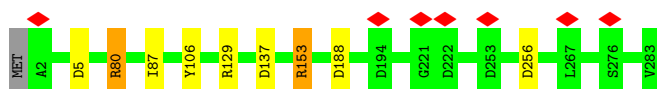
- Molecule 1: Tail tube, gp19

Chain Jb:  10% 98%



- Molecule 1: Tail tube, gp19

Chain Jc:  96%



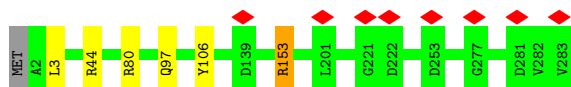
- Molecule 1: Tail tube, gp19

Chain Jd:  10% 96%



- Molecule 1: Tail tube, gp19

Chain Je:  98%



- Chain Lb: 

- Molecule 3: Tail collar fibers, gp4

- Molecule 3: Tail collar fibers, gp4

- Molecule 3: Tail collar fibers, gp4

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

Chain Lf: 29% 69%


[illegible]

Chain Lg: 

GLN	ALA	LEU	TRP	MET
TYR	CYS	ASN	ASP	T2
THR	VAL	GLU	ASP	
ALA	GLY	LEU	ILE	T36
ILE	ALA	ALA	ASP	
GLY	ASP	ALA	ASP	Y65
THR	SER	ALA	LYS	
LYS	ARG	LEU	PRO	P89
ASP	LEU	GLY	SER	
SER	SER	ASP	THR	A107
ASN	ASN	ASP	PHE	
THR	THR	PRO	THR	
ILE	THR	ASN	PRO	P110
TYR	ARG	PHE	SER	SER
LEU	PRO	ALA	SER	ALA
ARG	THR	THR	HIS	ASP
THR	ASP	THR	THR	TRP
ALA	GLY	VAL	HIS	ASP
	SER	ALA	SER	ALA
	VAL	SER	ILE	LEU
	THR	GLN	ALA	LEU
	ASN	ILE	ASN	ASN
	ALA	GLY	VAL	VAL
	LYS	ALA	THR	PRO
	VAL	LYS	GLY	SER
	ALA	ALA	LEU	GLU
	SER	ASP	GLN	PHE
	GLY	LYS	ASP	PRO
	ALA	ALA	LEU	PRO
	ILE	THR	LEU	SER
	GLY	THR	ASP	ALA
	LEU	ILE	GLU	HIS
	LEU	THR	LYS	ASP
	SER	ALA	LEU	HIS
	LYS	GLY	ASP	VAL
	ALA	GLY	ALA	ALA
	THR	LEU	ALA	ASP
	GLY	THR	VAL	VAL
	TYR	GLY	ASP	THR
	VAL	GLY	ALA	ASP
	ALA	GLY	ARG	LEU
	SER	LEU	SER	SER
	ASP	SER	LEU	ALA
	ASN	ALA	GLY	ILE
	SER	ASN	THR	ALA
	GLY	ARG	ALA	TYR
	ARG	THR	LEU	LEU
	THR	ASN	VAL	ALA
	LEU	VAL	ASP	SER
	THR	SER	SER	ASN
	ILE	PHE	ALA	PRO
	TRP	GLY	PRO	GLU
	VAL	THR	SER	ALA
	GLY	SER	THR	GLY
	THR	SER	LEU	SER
	GLU	THR	ASP	VAL
	ALA	THR	THR	ALA

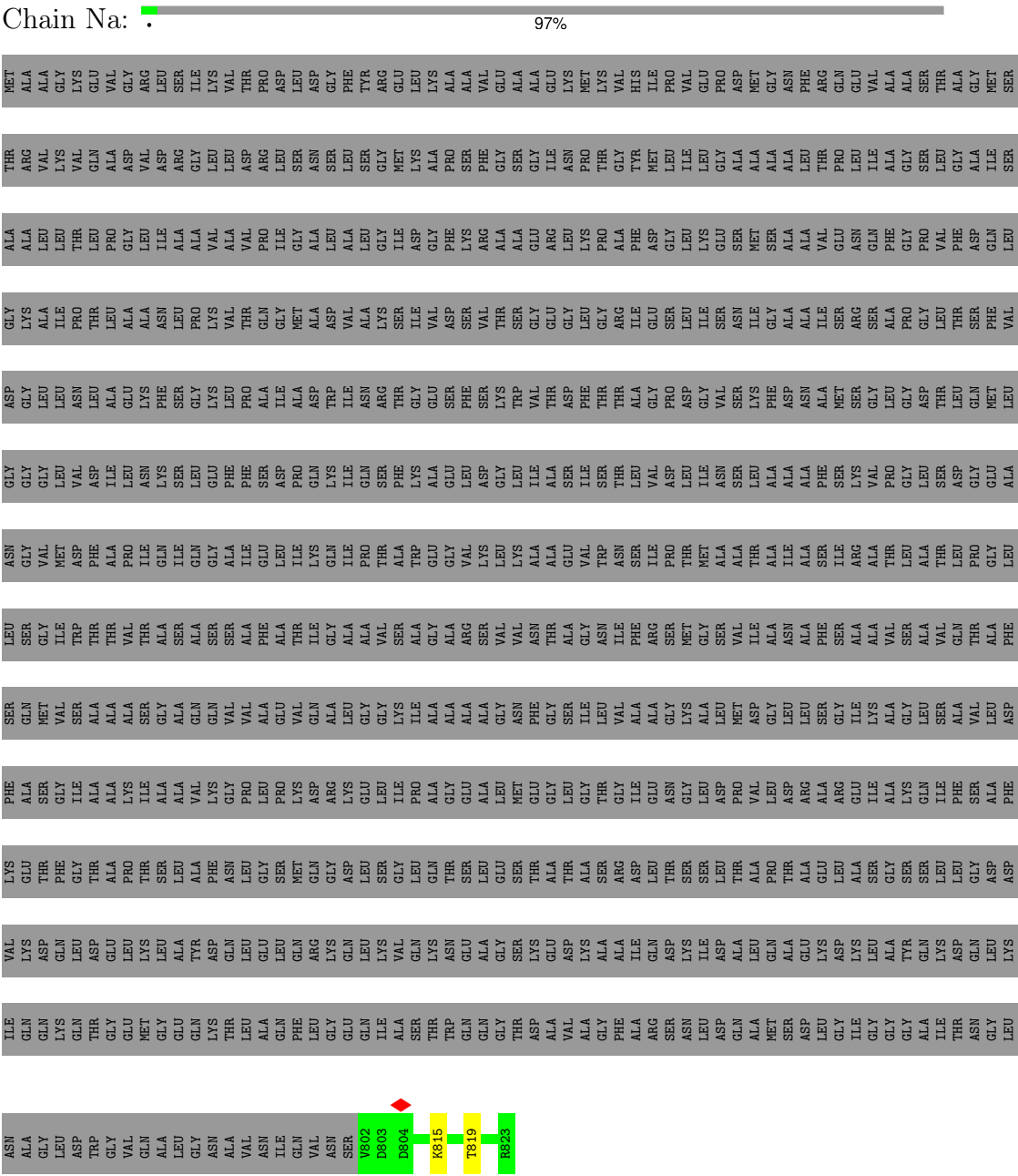
- [illegible]

- [illegible]

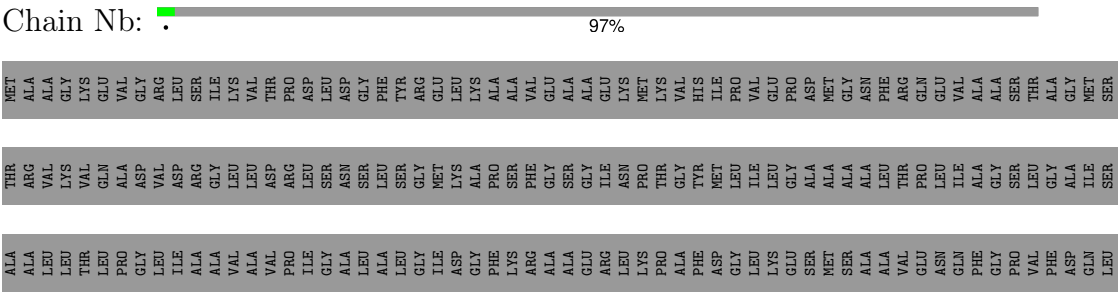
- Chain Ma:  94%

- Chain Mb: 95% ..

● Molecule 5: Tapemeasure protein



● Molecule 5: Tapemeasure protein





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

- Chain 0a:  97% 3%

ME1	PRO	ALA	PRO	A5	R25	L37	Y45	I83	R92	R108	M109	R116	V122	I245	R311	E357	E577	I580	I599	LEU
-----	-----	-----	-----	----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	-----

- Chain Ob:

[illegible]

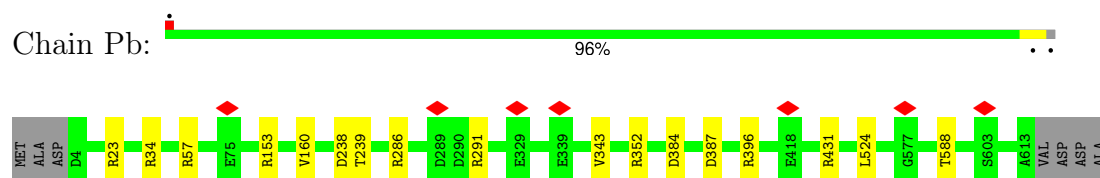
- Chain Oc: 97% ..

MET
PRO
ALA
PRO
A5
Q26
Y45
R48
T66
S70
H95
R108
E265
R311
L406
R435
R496
R523
E575
P576
E577
I599

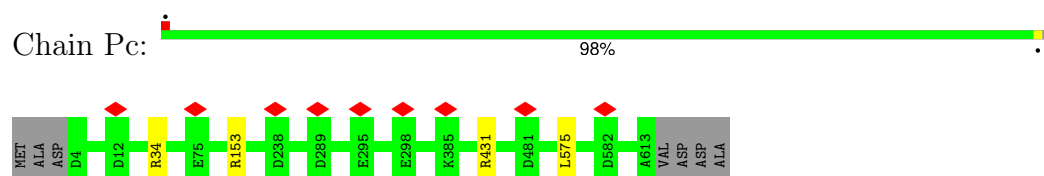
- Chain Pa:  97% ..

ASP	ASP
ALA	ALA
D4	MET
D21	ASP
R34	ALA
H72	ASP
E75	ALA
E94	ASP
D112	ASP
R153	ASP
V160	ASP
D175	ASP
N219	ASP
D238	ASP
N241	ASP
I253	ASP
D289	ASP
G312	ASP
S315	ASP
E329	ASP
R352	ASP
D360	ASP
K385	ASP
D392	ASP
E418	ASP
L524	ASP
Y535	ASP
H550	ASP
A551	ASP
E578	ASP
A613	ASP
H613	ASP

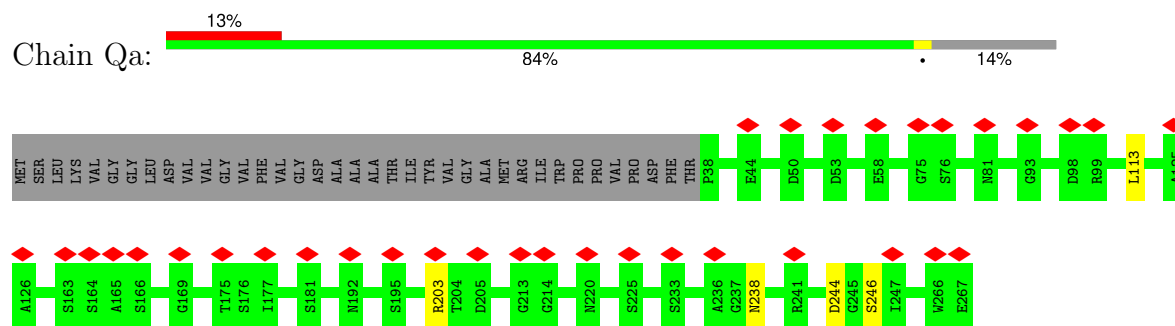
- Molecule 7: Tail spike, gp29



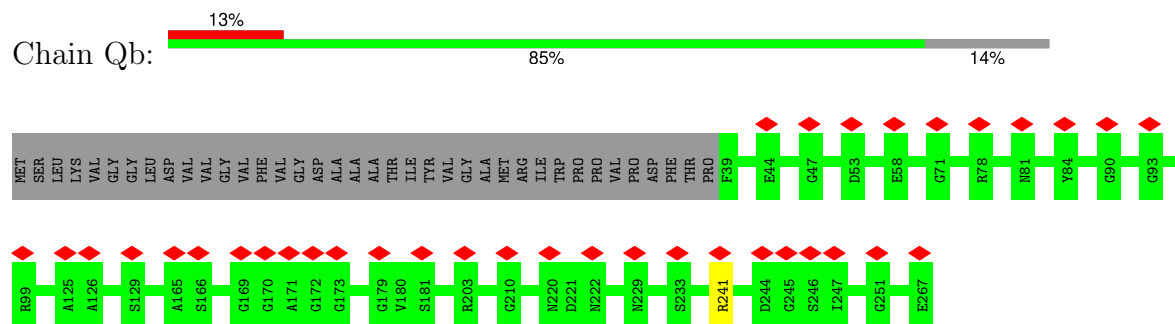
- Molecule 7: Tail spike, gp29



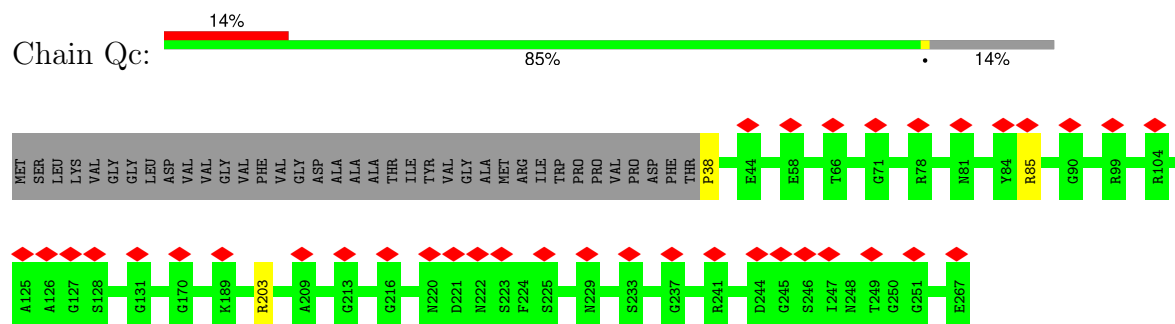
- Molecule 8: Tail wing brush, gp33



- Molecule 8: Tail wing brush, gp33



- Molecule 8: Tail wing brush, gp33



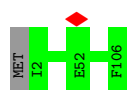
- Molecule 9: Tail wing arm, gp31

Chain Ra:  99%



- Molecule 9: Tail wing arm, gp31

Chain Rb:  99%



- Molecule 9: Tail wing arm, gp31

Chain Rc:  98%



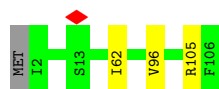
- Molecule 9: Tail wing arm, gp31

Chain Rd:  96%



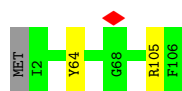
- Molecule 9: Tail wing arm, gp31

Chain Re:  96%



- Molecule 9: Tail wing arm, gp31

Chain Rf:  97%



- Molecule 10: Tail wing base, gp30

Chain Sa:  94%

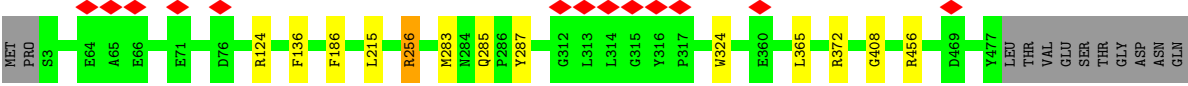


ASN
GLN
ILE
PRO
ALA
ASP
VAL
PRO
PHE
GLU
ILE

● 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 [i](#)

5.1 Standard geometry [i](#)

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.

All (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
6	Ob	311	ARG	NE-CZ-NH2	6.53	125.07	119.20
4	Mf	55	PHE	CA-CB-CG	6.52	120.32	113.80
9	Rd	105	ARG	NE-CZ-NH2	6.48	125.03	119.20
9	Re	105	ARG	NE-CZ-NH2	6.41	124.97	119.20
7	Pb	588	THR	CA-C-N	6.40	124.33	119.66
7	Pb	588	THR	C-N-CA	6.40	124.33	119.66
1	Jb	71	ARG	NE-CZ-NH2	6.32	124.88	119.20
7	Pc	431	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	Jc	137	ASP	CA-CB-CG	6.25	118.85	112.60
6	Ob	92	ARG	NE-CZ-NH2	6.22	124.80	119.20
3	Lg	36	THR	N-CA-C	6.19	120.14	112.59
6	Oc	311	ARG	NE-CZ-NH2	6.14	124.72	119.20
10	Sb	366	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	Jf	71	ARG	NE-CZ-NH2	6.10	124.69	119.20
10	Sa	256	ARG	NE-CZ-NH2	6.06	124.66	119.20
4	Me	255	ARG	NE-CZ-NH2	6.01	124.61	119.20
9	Rf	105	ARG	NE-CZ-NH2	6.00	124.60	119.20
4	Ma	155	ASP	CA-CB-CG	5.97	118.57	112.60
6	Oa	311	ARG	NE-CZ-NH2	5.97	124.57	119.20
7	Pb	387	ASP	CA-CB-CG	5.96	118.56	112.60
6	Oa	25	ARG	NE-CZ-NH2	5.93	124.53	119.20
7	Pa	219	ASN	N-CA-CB	-5.91	102.17	111.39
1	Jd	48	ASP	CA-CB-CG	5.91	118.51	112.60
4	Mc	391	GLU	N-CA-CB	5.90	118.67	110.17
6	Ob	543	ASP	CA-C-N	5.89	125.56	119.56
6	Ob	543	ASP	C-N-CA	5.89	125.56	119.56
10	Sc	256	ARG	NE-CZ-NH2	5.89	124.50	119.20
10	Sb	256	ARG	NE-CZ-NH2	5.86	124.47	119.20
4	Mb	649	PRO	N-CA-CB	5.82	106.45	103.19
6	Oc	48	ARG	NE-CZ-NH2	5.82	124.44	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Qc	38	PRO	CA-N-CD	-5.81	103.87	112.00
1	Ja	129	ARG	NE-CZ-NH2	5.79	124.41	119.20
7	Pa	352	ARG	NE-CZ-NH2	5.79	124.41	119.20
4	Mf	676	ARG	NE-CZ-NH2	5.79	124.41	119.20
3	Ld	10	ARG	NE-CZ-NH2	5.77	124.39	119.20
10	Sa	457	ASP	CA-CB-CG	5.76	118.36	112.60
4	Ma	591	ASP	CA-CB-CG	5.73	118.33	112.60
3	Ld	76	ALA	N-CA-C	5.73	118.30	111.71
6	Oa	92	ARG	NE-CZ-NH2	5.72	124.35	119.20
6	Ob	25	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	Je	3	LEU	N-CA-C	5.69	117.17	110.97
4	Md	133	ARG	NE-CZ-NH2	5.69	124.32	119.20
3	La	10	ARG	NE-CZ-NH2	5.69	124.32	119.20
6	Ob	116	ARG	NE-CZ-NH2	5.68	124.31	119.20
4	Ma	114	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	Je	80	ARG	NE-CZ-NH2	5.67	124.30	119.20
7	Pa	153	ARG	NE-CZ-NH2	5.66	124.30	119.20
3	Lb	41	ARG	NE-CZ-NH2	5.64	124.28	119.20
6	Oc	108	ARG	NE-CZ-NH2	5.63	124.27	119.20
10	Sc	456	ARG	NE-CZ-NH2	5.62	124.25	119.20
6	Oc	496	ARG	NE-CZ-NH2	5.62	124.25	119.20
7	Pc	34	ARG	NE-CZ-NH2	5.61	124.25	119.20
4	Ma	255	ARG	NE-CZ-NH2	5.61	124.25	119.20
7	Pb	286	ARG	NE-CZ-NH2	5.61	124.25	119.20
3	Le	41	ARG	NE-CZ-NH2	5.60	124.24	119.20
4	Md	676	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	Kc	40	ARG	NE-CZ-NH2	5.58	124.22	119.20
6	Oc	435	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	Jc	80	ARG	NE-CZ-NH2	5.57	124.22	119.20
3	Lh	93	SER	N-CA-C	5.57	119.94	113.20
7	Pb	23	ARG	NE-CZ-NH2	5.55	124.20	119.20
6	Ob	95	HIS	CB-CG-CD2	-5.55	123.98	131.20
4	Md	255	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	Ja	80	ARG	NE-CZ-NH2	5.53	124.18	119.20
4	Mc	564	ASP	CA-CB-CG	5.53	118.13	112.60
10	Sc	365	LEU	CA-C-N	5.52	128.23	120.28
10	Sc	365	LEU	C-N-CA	5.52	128.23	120.28
4	Ma	133	ARG	NE-CZ-NH2	5.51	124.16	119.20
7	Pb	153	ARG	NE-CZ-NH2	5.51	124.16	119.20
6	Ob	397	ASN	CA-CB-CG	5.49	118.09	112.60
3	Lc	41	ARG	NE-CZ-NH2	5.48	124.13	119.20
7	Pb	352	ARG	NE-CZ-NH2	5.47	124.12	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Ob	108	ARG	NE-CZ-NH2	5.46	124.11	119.20
3	Lb	12	VAL	CB-CA-C	-5.46	104.08	112.05
4	Mf	255	ARG	NE-CZ-NH2	5.43	124.09	119.20
4	Mb	67	ARG	NE-CZ-NH2	5.43	124.09	119.20
4	Md	383	ARG	NE-CZ-NH2	5.42	124.08	119.20
7	Pb	34	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	Jf	138	ASN	CA-CB-CG	5.42	118.02	112.60
8	Qc	203	ARG	NE-CZ-NH2	5.41	124.07	119.20
4	Mf	401	PRO	CA-C-N	5.41	129.25	120.60
4	Mf	401	PRO	C-N-CA	5.41	129.25	120.60
7	Pc	153	ARG	NE-CZ-NH2	5.40	124.06	119.20
6	Oa	108	ARG	NE-CZ-NH2	5.40	124.06	119.20
6	Oa	116	ARG	NE-CZ-NH2	5.39	124.05	119.20
4	Mf	68	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	Jc	188	ASP	CA-CB-CG	5.38	117.98	112.60
3	Lh	41	ARG	NE-CZ-NH2	5.38	124.04	119.20
2	Kc	25	ASP	CA-CB-CG	5.38	117.98	112.60
6	Ob	248	ARG	NE-CZ-NH2	5.38	124.04	119.20
7	Pa	315	SER	CA-C-N	5.38	125.09	119.82
7	Pa	315	SER	C-N-CA	5.38	125.09	119.82
4	Me	456	ARG	NE-CZ-NH2	5.38	124.04	119.20
10	Sb	259	ARG	NE-CZ-NH2	5.37	124.03	119.20
4	Mb	336	ARG	NE-CZ-NH2	5.36	124.03	119.20
4	Mf	114	ARG	NE-CZ-NH2	5.36	124.03	119.20
7	Pb	396	ARG	NE-CZ-NH2	5.35	124.02	119.20
4	Mc	456	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	Ja	226	ASN	CA-CB-CG	5.35	117.95	112.60
1	Jd	186	GLU	CB-CA-C	-5.34	102.86	110.34
6	Ob	48	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	Jd	147	ARG	NE-CZ-NH2	5.34	124.00	119.20
8	Qc	85	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	Jf	281	ASP	CA-CB-CG	5.33	117.93	112.60
10	Sc	372	ARG	NE-CZ-NH2	5.32	123.98	119.20
7	Pa	34	ARG	NE-CZ-NH2	5.31	123.98	119.20
4	Mb	255	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	Je	44	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	Jb	48	ASP	CA-CB-CG	5.27	117.87	112.60
4	Ma	673	ARG	NE-CZ-NH2	5.26	123.93	119.20
4	Mc	478	PHE	CA-CB-CG	5.25	119.05	113.80
10	Sa	337	SER	N-CA-C	5.24	119.52	113.18
4	Mc	438	ASP	CA-CB-CG	5.23	117.83	112.60
3	Lb	91	ASP	CA-CB-CG	5.22	117.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Lh	76	ALA	N-CA-C	5.22	117.42	110.53
4	Ma	127	ASP	CA-CB-CG	5.20	117.80	112.60
1	Jd	71	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Jb	80	ARG	NE-CZ-NH2	5.19	123.87	119.20
3	Le	10	ARG	NE-CZ-NH2	5.19	123.87	119.20
10	Sc	124	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Jc	5	ASP	CA-CB-CG	5.18	117.78	112.60
4	Ma	433	ASP	CA-CB-CG	5.18	117.78	112.60
3	Ld	41	ARG	NE-CZ-NH2	5.17	123.86	119.20
4	Mf	456	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Jf	129	ARG	NE-CZ-NH2	5.16	123.84	119.20
4	Md	649	PRO	N-CA-CB	5.15	106.08	103.19
6	Ob	375	ASP	N-CA-CB	-5.15	102.40	109.97
6	Ob	319	ASP	CA-CB-CG	5.14	117.75	112.60
4	Mf	680	ARG	N-CA-C	5.13	114.20	108.25
10	Sa	186	PHE	CA-CB-CG	5.12	118.92	113.80
1	Jd	185	ILE	CA-C-N	5.11	129.86	121.58
1	Jd	185	ILE	C-N-CA	5.11	129.86	121.58
4	Mf	522	ASP	CA-CB-CG	5.11	117.71	112.60
1	Je	97	GLN	OE1-CD-NE2	-5.10	117.50	122.60
4	Md	114	ARG	NE-CZ-NH2	5.10	123.79	119.20
9	Rc	80	ASP	CA-CB-CG	5.10	117.70	112.60
7	Pb	238	ASP	CA-CB-CG	5.10	117.70	112.60
4	Mf	272	GLN	OE1-CD-NE2	-5.09	117.51	122.60
4	Md	648	ILE	CA-C-N	5.09	123.37	119.66
4	Md	648	ILE	C-N-CA	5.09	123.37	119.66
4	Mb	648	ILE	CA-C-N	5.09	123.37	119.66
4	Mb	648	ILE	C-N-CA	5.09	123.37	119.66
10	Sc	186	PHE	CA-CB-CG	5.08	118.89	113.80
1	Jc	256	ASP	CA-CB-CG	5.08	117.68	112.60
4	Mc	496	ASP	CA-CB-CG	5.08	117.68	112.60
7	Pa	238	ASP	CA-CB-CG	5.08	117.68	112.60
8	Qb	241	ARG	NE-CZ-NH2	5.08	123.77	119.20
3	Lb	10	ARG	NE-CZ-NH2	5.08	123.77	119.20
4	Mb	114	ARG	NE-CZ-NH2	5.07	123.77	119.20
4	Ma	59	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	Mc	114	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	Mb	136	GLU	N-CA-CB	-5.06	102.50	110.30
4	Md	525	ARG	NE-CZ-NH2	5.06	123.76	119.20
10	Sb	467	ASP	CA-CB-CG	5.06	117.66	112.60
8	Qa	203	ARG	NE-CZ-NH2	5.06	123.75	119.20
8	Qa	246	SER	N-CA-C	5.06	116.88	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Me	638	ARG	NE-CZ-NH2	5.05	123.75	119.20
6	Ob	541	TYR	CA-C-N	5.05	124.71	119.56
6	Ob	541	TYR	C-N-CA	5.05	124.71	119.56
1	Jd	5	ASP	CA-CB-CG	5.04	117.64	112.60
4	Mb	572	ARG	NE-CZ-NH2	5.04	123.73	119.20
7	Pb	291	ARG	NE-CZ-NH2	5.04	123.73	119.20
4	Me	114	ARG	NE-CZ-NH2	5.03	123.73	119.20
10	Sb	301	GLN	OE1-CD-NE2	-5.03	117.57	122.60
4	Ma	267	ARG	NE-CZ-NH2	5.03	123.73	119.20
6	Oc	523	ARG	NE-CZ-NH2	5.02	123.72	119.20
3	Lf	41	ARG	NE-CZ-NH2	5.01	123.71	119.20
7	Pa	21	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (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
3	La	65	TYR	Sidechain
3	Lb	65	TYR	Sidechain
3	Lc	41	ARG	Sidechain
3	Ld	41	ARG	Sidechain
3	Le	41	ARG	Sidechain
3	Le	65	TYR	Sidechain
3	Lf	10	ARG	Sidechain
3	Lf	41	ARG	Sidechain
3	Lg	65	TYR	Sidechain
4	Ma	525	ARG	Sidechain
4	Ma	606	ARG	Sidechain
4	Ma	676	ARG	Sidechain
4	Mb	119	ARG	Sidechain
4	Mb	240	TYR	Sidechain
4	Mb	67	ARG	Sidechain
4	Mc	119	ARG	Sidechain
4	Mc	240	TYR	Sidechain
4	Mc	525	ARG	Sidechain
4	Mc	606	ARG	Sidechain
4	Me	240	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	Me	307	ARG	Sidechain
4	Me	525	ARG	Sidechain
4	Me	606	ARG	Sidechain
4	Me	676	ARG	Sidechain
5	Nc	822	ARG	Sidechain
6	Oc	45	TYR	Sidechain
7	Pa	535	TYR	Sidechain
7	Pb	431	ARG	Sidechain
7	Pb	57	ARG	Sidechain
9	Rd	105	ARG	Sidechain
9	Rf	64	TYR	Sidechain
10	Sa	366	ARG	Sidechain
10	Sb	256	ARG	Sidechain
10	Sc	256	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
10:Sb:401:LEU:HD11	10:Sb:418:GLN:HE21	1.74	0.51
4:Mc:86:LEU:C	4:Mc:86:LEU:HD23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Qa:113:LEU:C	8:Qa:113:LEU:HD13	2.37	0.49
10:Sc:136:PHE:HA	10:Sc:283:MET:HE1	1.95	0.47
4:Md:555:LEU:H	4:Md:555:LEU:HD22	1.79	0.47
10:Sc:324:TRP:CE2	10:Sc:408:GLY:HA2	2.50	0.47
5:Na:819:THR:HG22	6:Oc:66:THR:O	2.17	0.45
4:Md:225:LEU:H	4:Md:225:LEU:HD23	1.81	0.44
5:Nb:813:VAL:HG11	6:Oa:580:ILE:HG21	2.00	0.43
7:Pa:550:HIS:CG	7:Pa:551:TRP:H	2.38	0.42
10:Sc:283:MET:HE3	10:Sc:287:TYR:HB2	2.01	0.42
10:Sa:136:PHE:HA	10:Sa:283:MET:HE1	2.02	0.42
4:Ma:682:TRP:CE3	4:Mf:86:LEU:HD13	2.55	0.41
4:Mc:86:LEU:HD12	4:Mc:133:ARG:HD3	2.02	0.41
4:Mb:86:LEU:HD12	4:Mb:133:ARG:HD3	2.02	0.41
6:Ob:317:ALA:HB3	6:Ob:322:THR:HG23	2.02	0.41
1:Jc:106:TYR:CE2	1:Jc:153:ARG:HD3	2.55	0.41
4:Mc:271:VAL:HG22	4:Mc:572:ARG:HG2	2.02	0.41
4:Mc:555:LEU:H	4:Mc:555:LEU:HD22	1.84	0.41
4:Mf:87:ARG:HD3	4:Mf:87:ARG:HA	1.94	0.41
1:Je:106:TYR:CE2	1:Je:153:ARG:HD3	2.56	0.40
6:Ob:565:LYS:HA	6:Ob:565:LYS:HE2	2.03	0.40
6:Oc:406:LEU:C	6:Oc:406:LEU:HD13	2.46	0.40
3:Ld:29:GLN:HB2	3:Li:79:TRP:CE2	2.57	0.40
4:Mb:175:TRP:HA	4:Mb:176:PRO:C	2.46	0.40
4:Me:213:LYS:HA	4:Me:214:PRO:HD3	1.98	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ja	104	GLU
1	Ja	226	ASN
1	Jc	87	ILE
1	Jd	5	ASP
1	Jd	218	LYS
1	Jf	55	GLU
1	Jf	57	ASP
1	Jf	105	LEU
1	Jf	138	ASN
2	Kb	65	ARG
2	Kc	50	LEU
3	La	27	LEU
3	La	49	LEU
3	Lb	12	VAL
3	Lb	43	ASN
3	Lb	96	LEU
3	Le	97	LEU
3	Lf	9	VAL
3	Lf	29	GLN
3	Lh	93	SER
3	Li	27	LEU
3	Li	30	GLN
3	Li	71	VAL
4	Ma	31	ILE
4	Ma	144	VAL
4	Ma	498	ASP
4	Ma	522	ASP
4	Ma	598	VAL
4	Ma	605	LEU

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Mol	Chain	Res	Type
4	Ma	624	GLU
4	Ma	631	SER
4	Mb	54	ASN
4	Mb	99	LYS
4	Mb	354	THR
4	Mb	555	LEU
4	Mb	685	GLU
4	Mc	41	LEU
4	Mc	70	LEU
4	Mc	82	ASP
4	Mc	144	VAL
4	Mc	201	ILE
4	Mc	364	ASP
4	Md	110	GLU
4	Md	222	LEU
4	Md	555	LEU
4	Md	574	THR
4	Md	668	GLN
4	Me	68	ARG
4	Me	70	LEU
4	Me	82	ASP
4	Me	144	VAL
4	Me	364	ASP
4	Me	498	ASP
4	Me	517	VAL
4	Me	522	ASP
4	Me	555	LEU
4	Mf	127	ASP
4	Mf	364	ASP
4	Mf	625	GLU
4	Mf	637	GLU
4	Mf	685	GLU
5	Na	815	LYS
5	Nb	823	ARG
5	Nc	822	ARG
6	Oa	37	LEU
6	Oa	45	TYR
6	Oa	122	VAL
6	Oa	245	ILE
6	Ob	44	ASP
6	Ob	45	TYR
6	Ob	125	GLU

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Mol	Chain	Res	Type
6	Ob	271	ILE
6	Ob	313	VAL
6	Ob	406	LEU
6	Oc	26	GLN
6	Oc	45	TYR
6	Oc	70	SER
6	Oc	406	LEU
7	Pa	160	VAL
7	Pa	241	ASN
7	Pa	418	GLU
7	Pa	524	LEU
7	Pb	160	VAL
7	Pb	239	THR
7	Pb	343	VAL
7	Pb	384	ASP
7	Pb	524	LEU
7	Pc	575	LEU
8	Qa	238	ASN
8	Qa	244	ASP
9	Rd	10	ASN
9	Rd	11	LEU
9	Re	62	ILE
9	Re	96	VAL
10	Sa	10	VAL
10	Sa	107	VAL
10	Sa	118	LYS
10	Sa	372	ARG
10	Sb	407	LEU
10	Sc	215	LEU
10	Sc	285	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	Jd	111	GLN
1	Jd	145	HIS
1	Jd	180	ASN
1	Jf	111	GLN
1	Jf	145	HIS
2	Ka	62	HIS
2	Kb	29	GLN
3	La	29	GLN

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Mol	Chain	Res	Type
3	Lb	108	ASN
3	Lc	20	GLN
3	Lc	43	ASN
3	Ld	20	GLN
3	Ld	43	ASN
3	Ld	108	ASN
3	Le	15	GLN
3	Lf	20	GLN
3	Lf	29	GLN
3	Lf	43	ASN
3	Lf	102	ASN
3	Lg	102	ASN
3	Li	39	GLN
4	Ma	18	ASN
4	Ma	54	ASN
4	Ma	138	ASN
4	Ma	361	ASN
4	Ma	421	ASN
4	Ma	436	ASN
4	Ma	440	ASN
4	Ma	452	HIS
4	Ma	646	HIS
4	Mb	54	ASN
4	Mb	62	ASN
4	Mb	138	ASN
4	Mb	199	ASN
4	Mb	542	GLN
4	Mc	54	ASN
4	Mc	138	ASN
4	Mc	193	ASN
4	Mc	199	ASN
4	Mc	262	GLN
4	Mc	273	GLN
4	Mc	330	ASN
4	Mc	390	ASN
4	Mc	436	ASN
4	Mc	539	ASN
4	Md	62	ASN
4	Me	26	ASN
4	Me	54	ASN
4	Me	81	ASN
4	Me	138	ASN

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Mol	Chain	Res	Type
4	Me	330	ASN
4	Me	436	ASN
4	Mf	62	ASN
4	Mf	532	GLN
4	Mf	542	GLN
5	Na	816	GLN
5	Nb	811	ASN
5	Nb	816	GLN
6	Oa	16	GLN
6	Oa	86	HIS
6	Ob	50	GLN
6	Ob	101	GLN
6	Ob	499	GLN
7	Pa	283	ASN
7	Pb	53	GLN
7	Pb	72	ASN
7	Pb	219	ASN
7	Pb	409	HIS
7	Pb	413	GLN
7	Pb	456	GLN
7	Pb	569	GLN
7	Pc	283	ASN
7	Pc	301	HIS
7	Pc	319	ASN
7	Pc	413	GLN
8	Qa	81	ASN
8	Qb	81	ASN
10	Sa	13	ASN
10	Sa	42	GLN
10	Sa	85	GLN
10	Sa	135	ASN
10	Sa	187	GLN
10	Sa	195	GLN
10	Sa	202	GLN
10	Sa	284	ASN
10	Sb	13	ASN
10	Sb	127	ASN
10	Sb	135	ASN
10	Sb	301	GLN
10	Sb	399	HIS
10	Sb	429	ASN
10	Sc	9	ASN

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Mol	Chain	Res	Type
10	Sc	13	ASN
10	Sc	18	ASN
10	Sc	85	GLN
10	Sc	135	ASN
10	Sc	147	ASN
10	Sc	187	GLN
10	Sc	284	ASN
10	Sc	285	GLN
10	Sc	301	GLN

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.

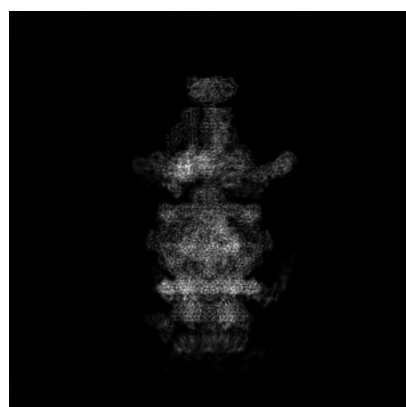
6 Map visualisation [i](#)

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.

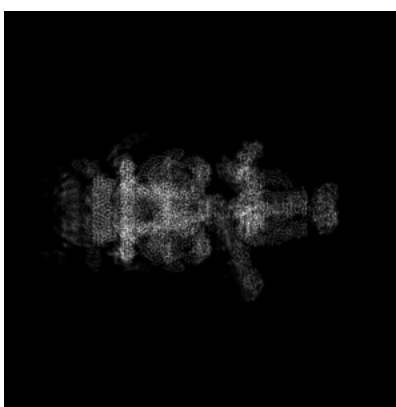
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

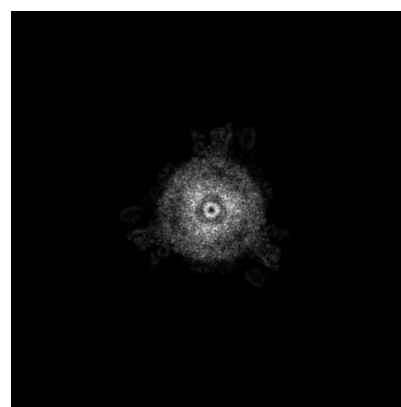
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

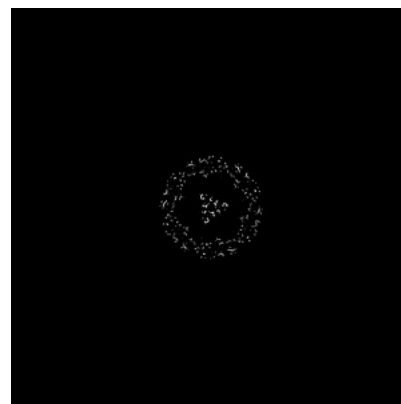
6.2.1 Primary map



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

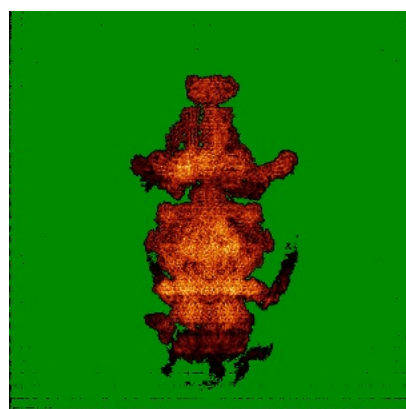


Z Index: 147

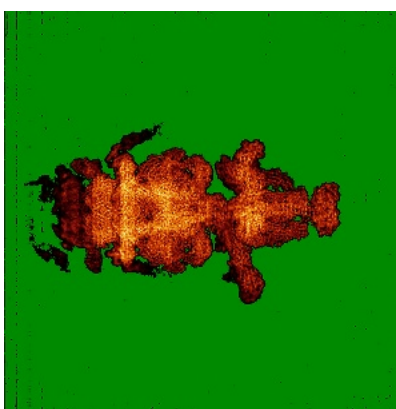
The images above show the largest variance slices of the map in three orthogonal directions.

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

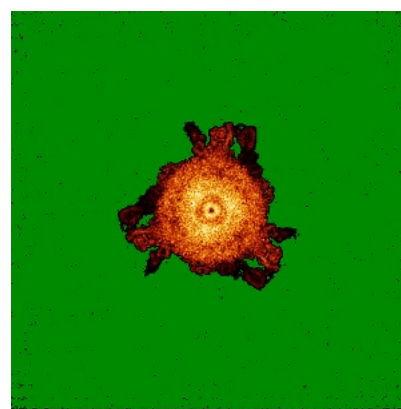
6.4.1 Primary map



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.

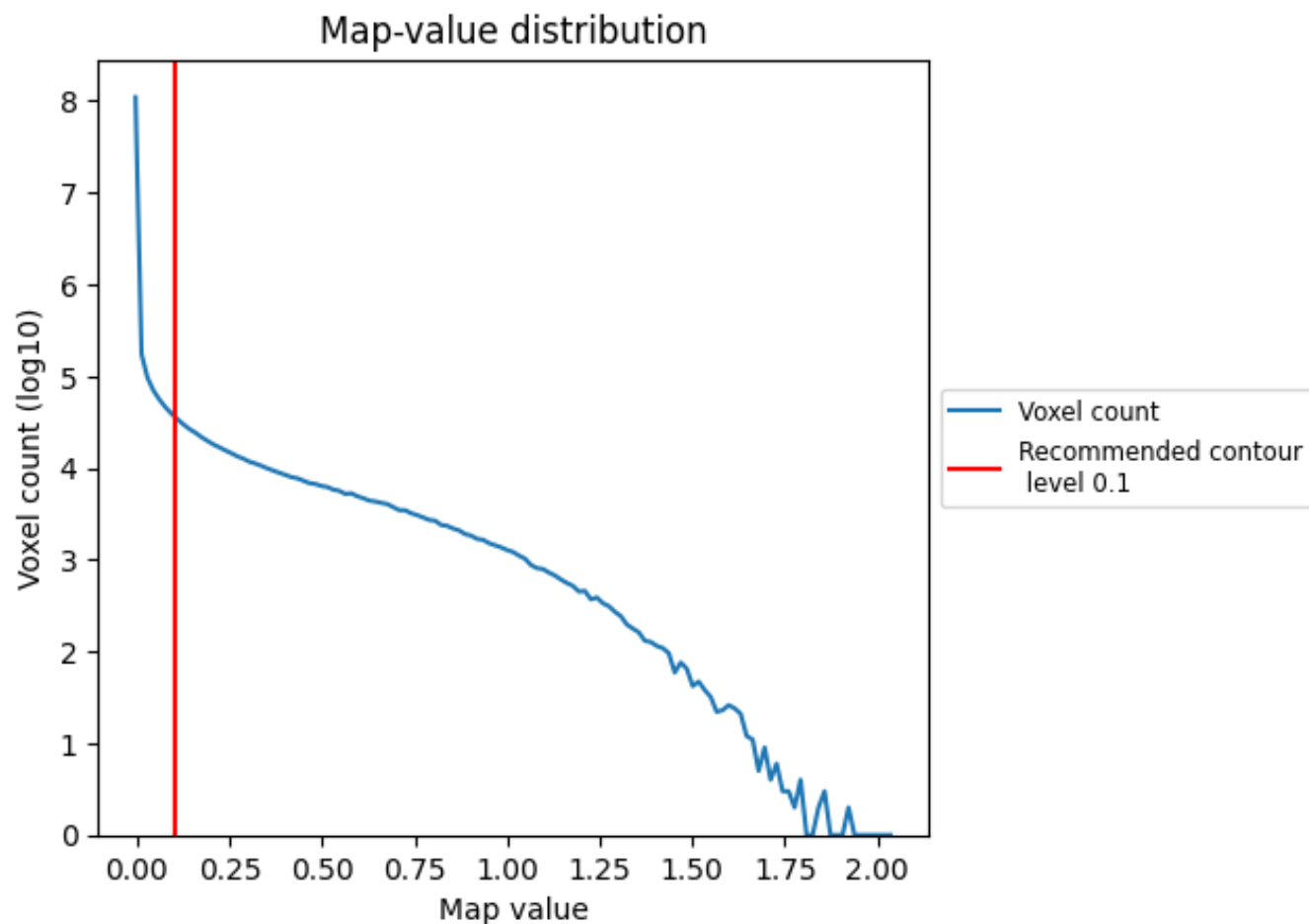
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

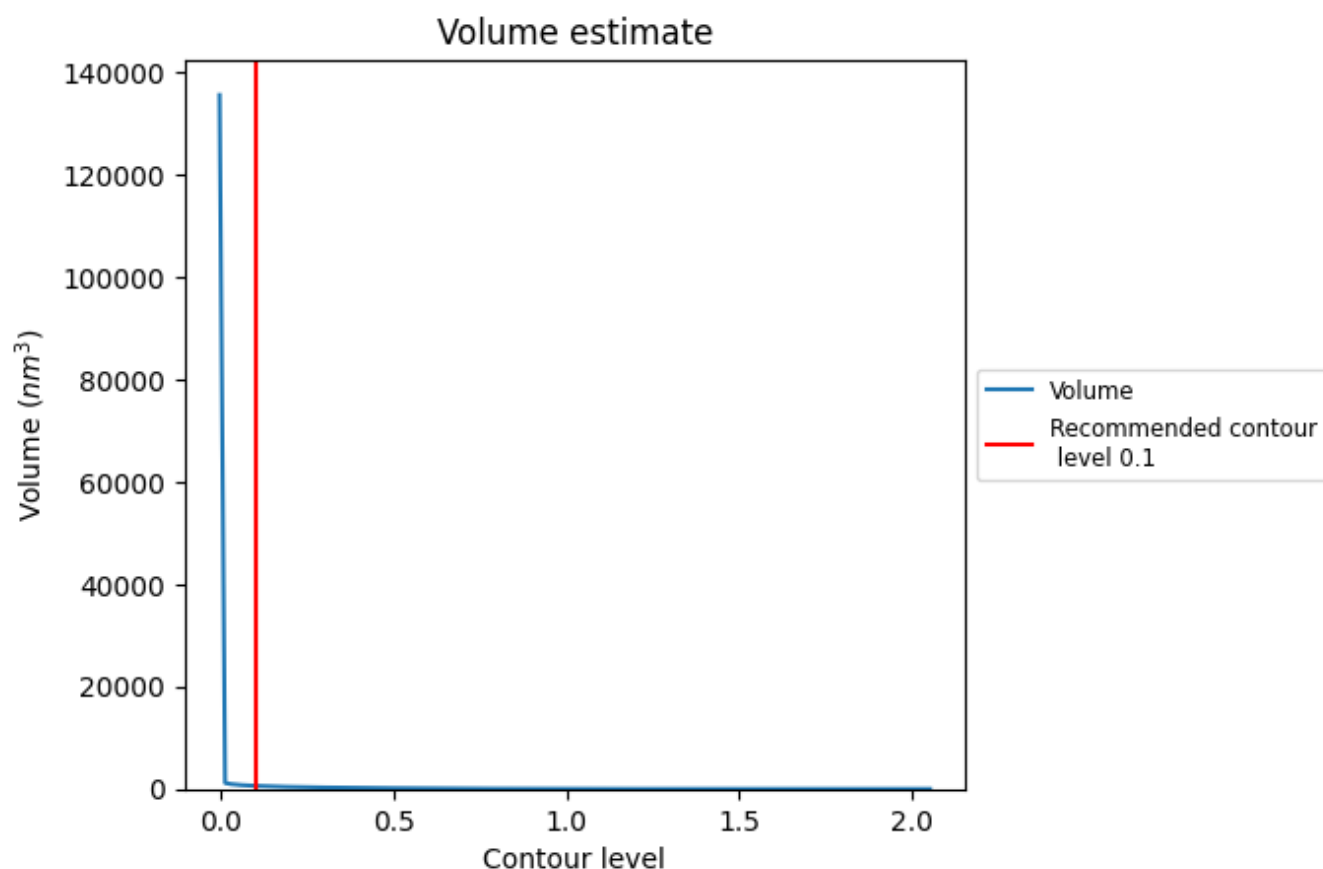
This section contains the results of statistical analysis of the map.

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.

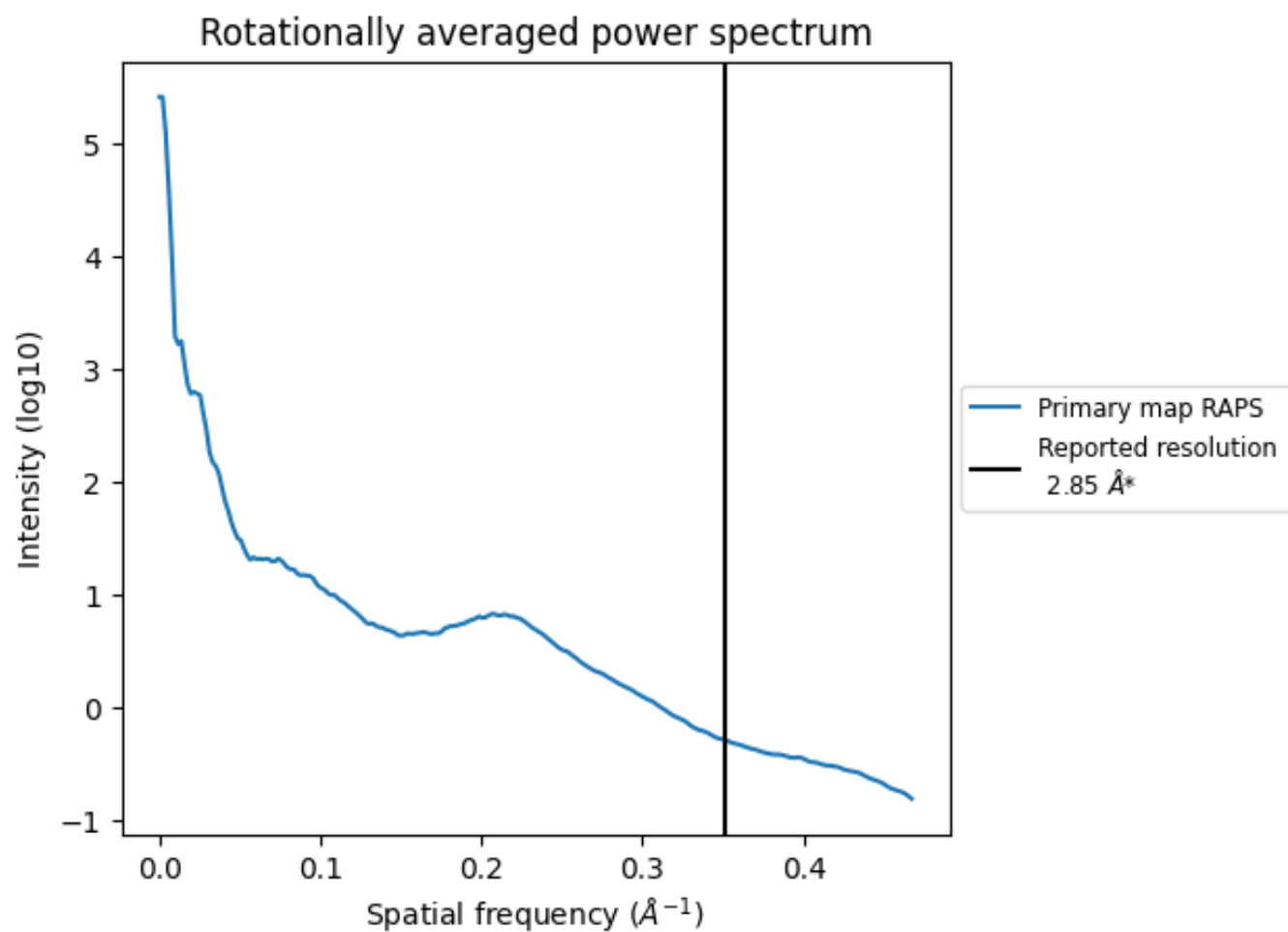
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 610 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⁻¹

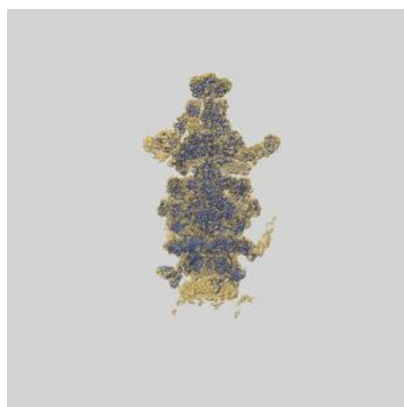
8 Fourier-Shell correlation ⓘ

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

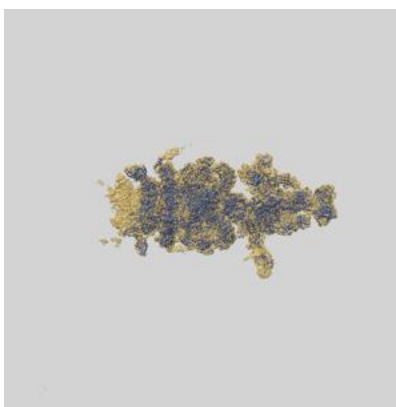
9 Map-model fit [i](#)

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](#).

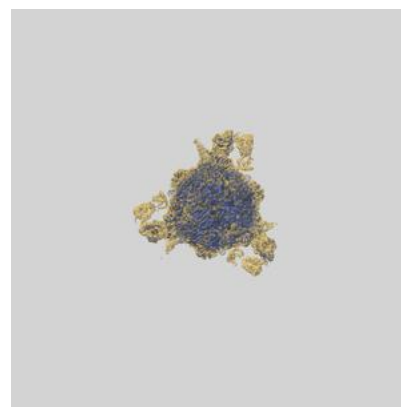
9.1 Map-model overlay [i](#)



X



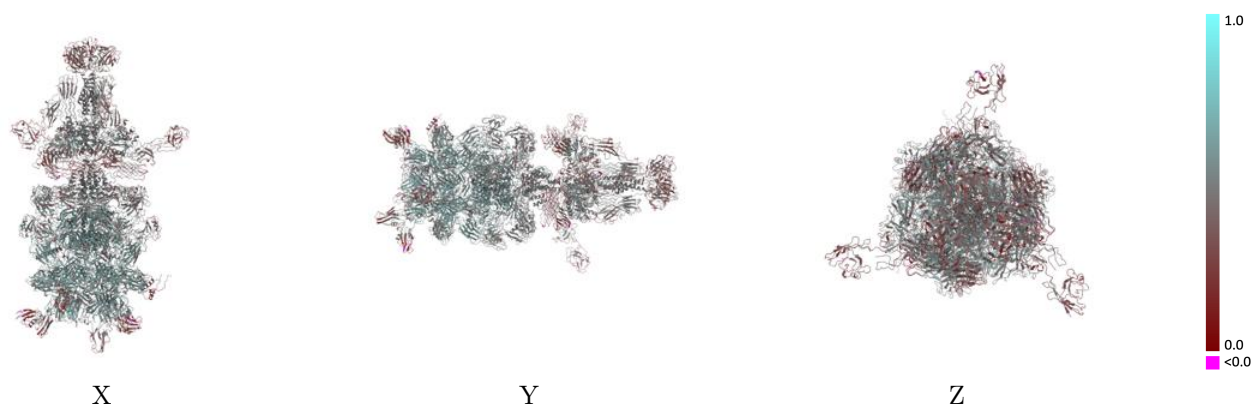
Y



Z

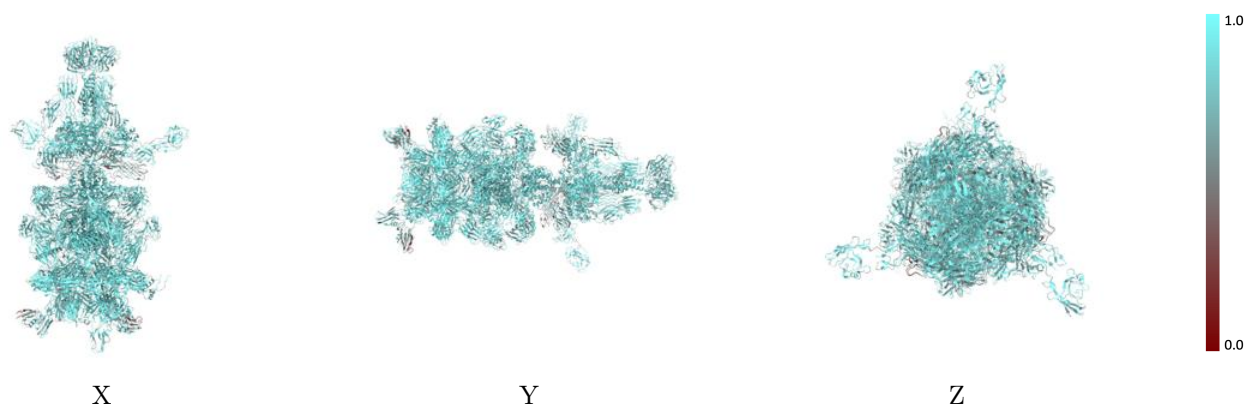
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



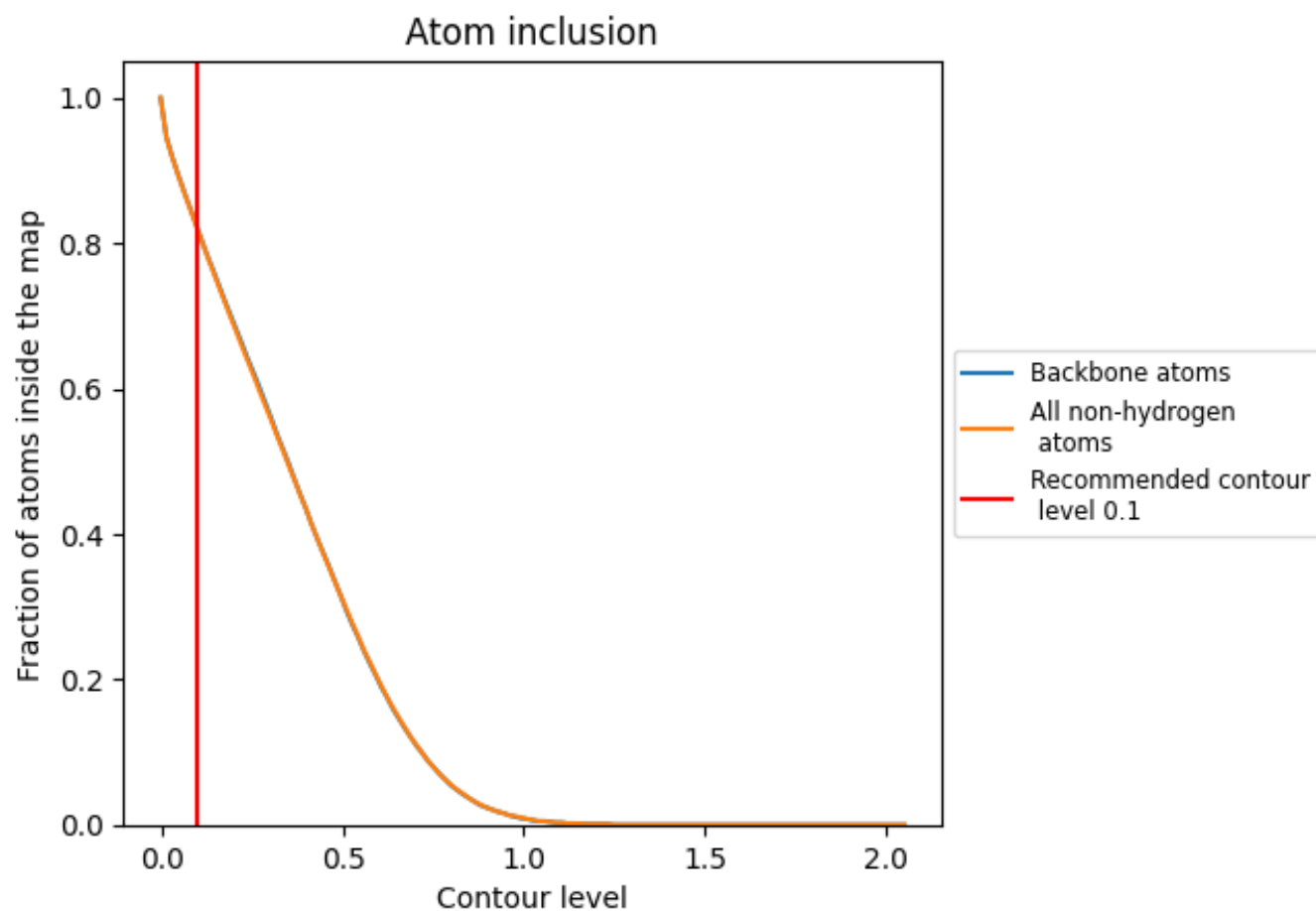
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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