



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 10:46 PM UTC

PDB ID : 8FQC / pdb_00008fqc
EMDB ID : EMD-29383
Title : Structure of baseplate with receptor binding complex of Agrobacterium phage Milano
Authors : Sonani, R.R.; Leiman, P.G.; Wang, F.; Kreutzberger, M.A.B.; Sebastian, A.; Esteves, N.C.; Kelly, R.J.; Scharf, B.; Egelman, E.H.
Deposited on : 2023-01-05
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

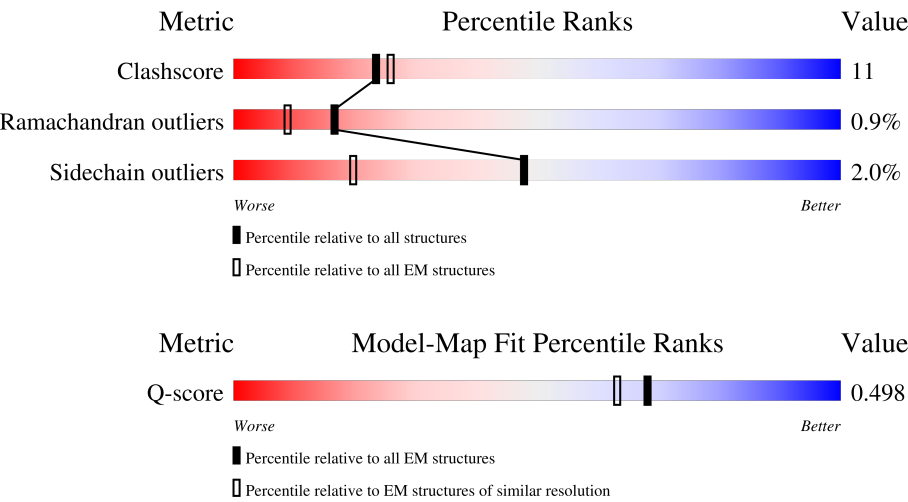
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



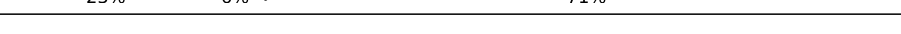
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	C1	457	
2	E1	136	
2	a1	136	
2	f1	136	

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Mol	Chain	Length	Quality of chain
2	g1	136	 82% 15% .
3	F1	396	 84% 14% ..
3	G1	396	 77% 20% ...
3	h1	396	 86% 12% ..
3	i1	396	 77% 21% ..
4	H1	178	 78% 21% .
4	j1	178	 78% 20% ..
5	I1	503	 77% 21% ..
5	K1	503	 74% 22% ..
5	k1	503	 74% 24% ..
5	m1	503	 72% 24% . .
6	J1	286	 74% 22% .
6	l1	286	 79% 18% .
7	P1	587	 22% 6% 72%
7	Q1	587	 23% 6% . 71%
7	R1	587	 22% 6% . 71%
7	r1	587	 21% 6% 72%
7	s1	587	 23% 5% . 71%
7	t1	587	 22% 7% 71%
8	S1	300	 28% 12% 60%
8	T1	300	 24% 16% 60%
8	V1	300	 26% 14% 60%
8	W1	300	 28% 12% 60%
8	X1	300	 28% 11% 60%
8	Y1	300	 30% 10% 60%

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Mol	Chain	Length	Quality of chain
8	u1	300	 28%11%60%
8	v1	300	 21%18%60%
8	w1	300	 28%11%60%
8	x1	300	 25%14%60%
8	y1	300	 27%13%60%
8	z1	300	 29%10%60%
9	U1	398	 85%13%...
9	e1	398	 81%16%..
10	A	188	 64%15%8%•11%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 66089 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Baseplate hub protein, gp26.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	326	Total	C	N	O	S	0	0
			2551	1610	434	500	7		

- Molecule 2 is a protein called Tail-tube, gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	a1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	f1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	g1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		

- Molecule 3 is a protein called Baseplate Wedge 2 protein, gp29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	G1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	h1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	i1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		

- Molecule 4 is a protein called Baseplate wedge 1, gp28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	j1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

- Molecule 5 is a protein called Tail sheath protein, gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	K1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		
5	k1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	m1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		

- Molecule 6 is a protein called Baseplate Wedge 3 protein, gp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		
6	l1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		

- Molecule 7 is a protein called Tail Spike protein, gp124.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	Q1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	R1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	r1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	s1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	t1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		

- Molecule 8 is a protein called Short Tail Fibers, gp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	T1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	V1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	W1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	X1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	Y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	v1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	w1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	x1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	u1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	z1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		

- Molecule 9 is a protein called Baseplate Centerpiece, gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		
9	e1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		

- Molecule 10 is a protein called Baseplate Central Spike, gp27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	168	Total	C	N	O	S	0	0
			1289	799	223	264	3		

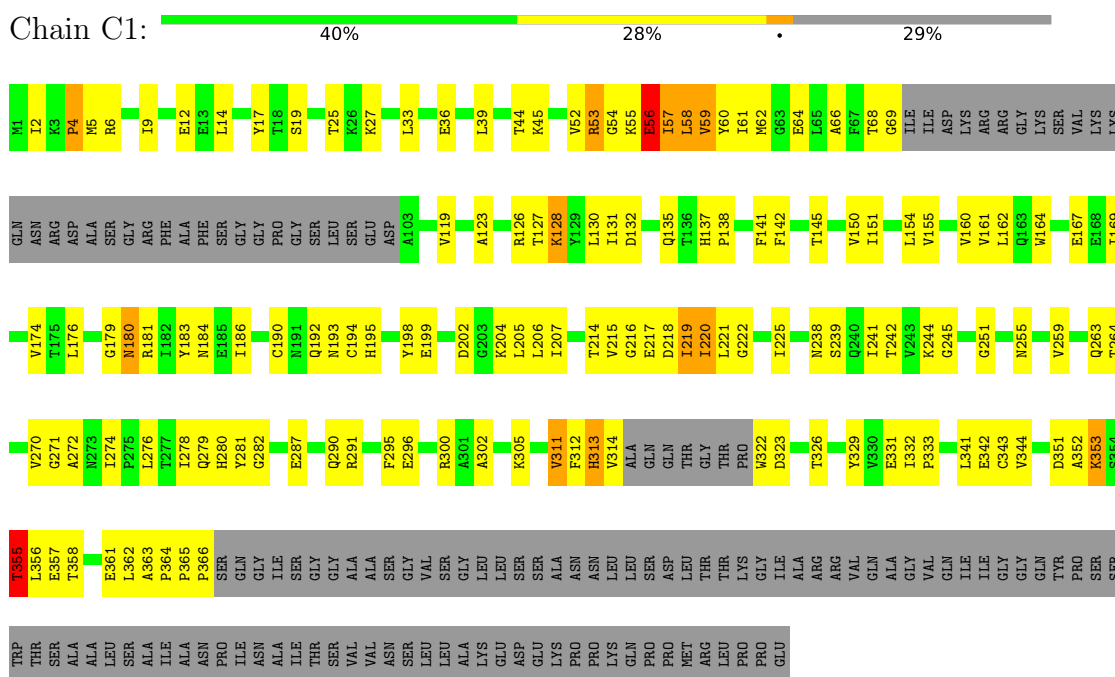
- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total 1	Fe 1	0

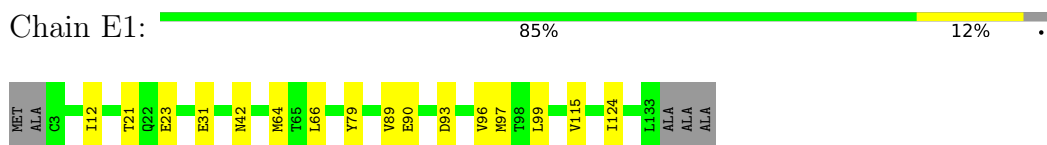
3 Residue-property plots [i](#)

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.

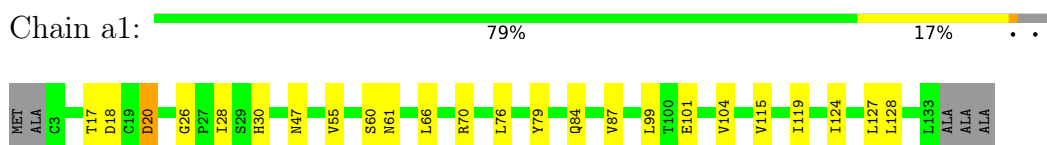
- Molecule 1: Baseplate hub protein, gp26



- Molecule 2: Tail-tube, gp21



- Molecule 2: Tail-tube, gp21



- Molecule 2: Tail-tube, gp21

Chain f1:  80% 16%



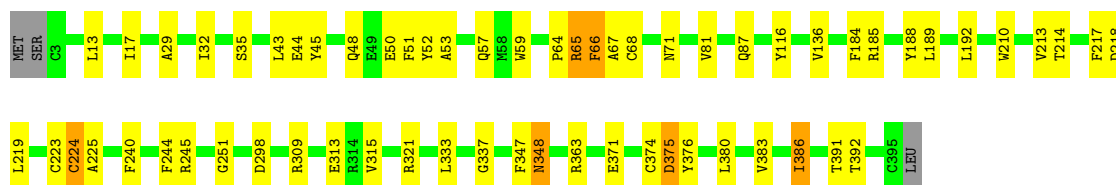
- Molecule 2: Tail-tube, gp21

Chain g1:  82% 15%



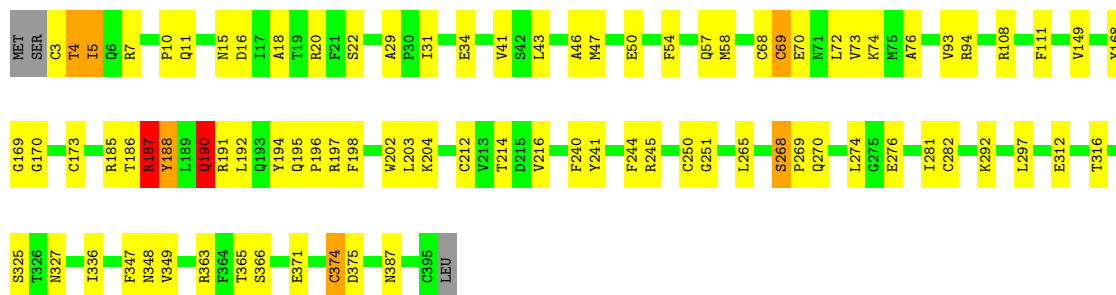
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain F1:  84% 14%



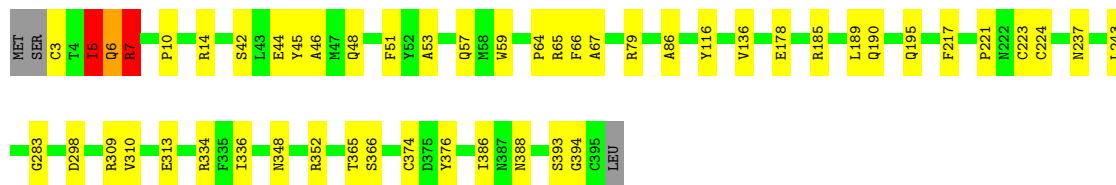
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain G1:  77% 20%



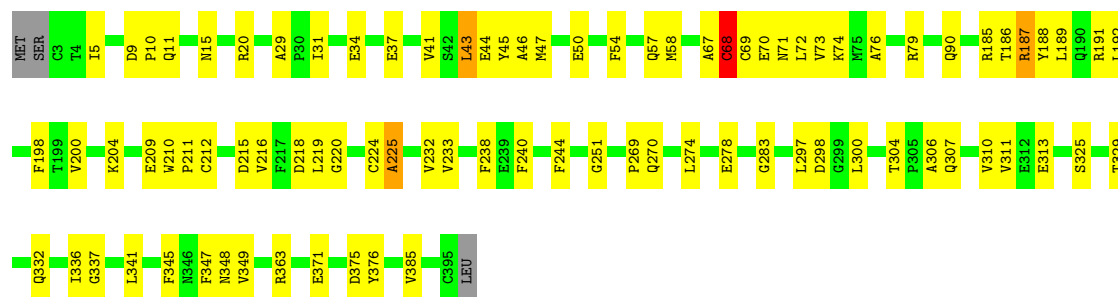
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain h1:  86% 12%



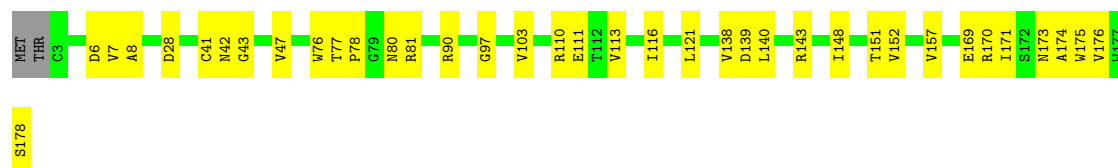
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain i1:  77% 21%



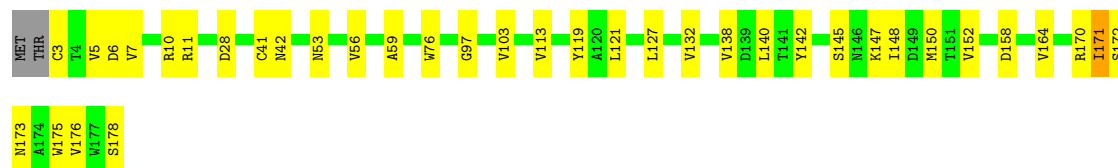
• Molecule 4: Baseplate wedge 1, gp28

Chain H1: 78% 21%



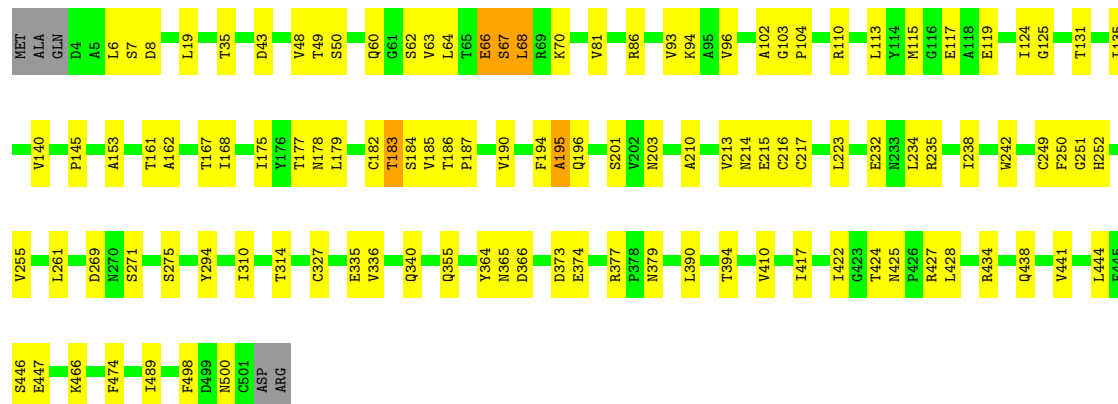
• Molecule 4: Baseplate wedge 1, gp28

Chain j1: 78% 20%



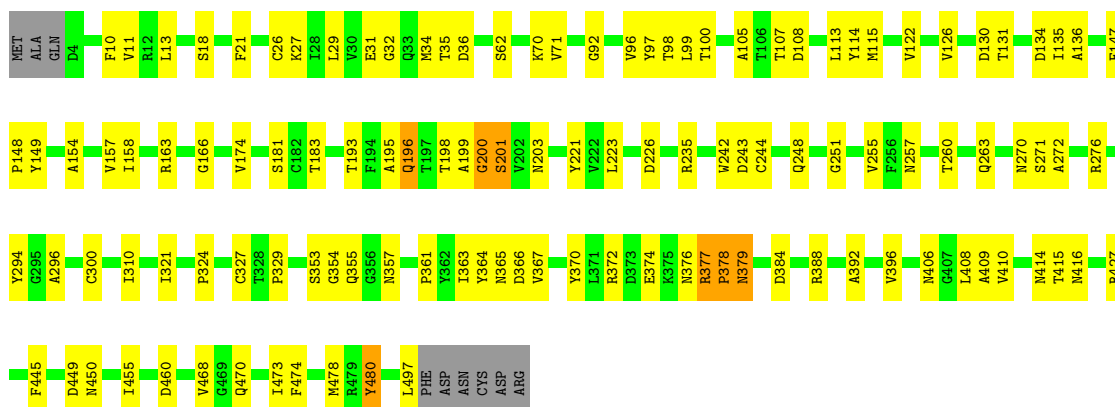
• Molecule 5: Tail sheath protein, gp20

Chain I1: 77% 21%



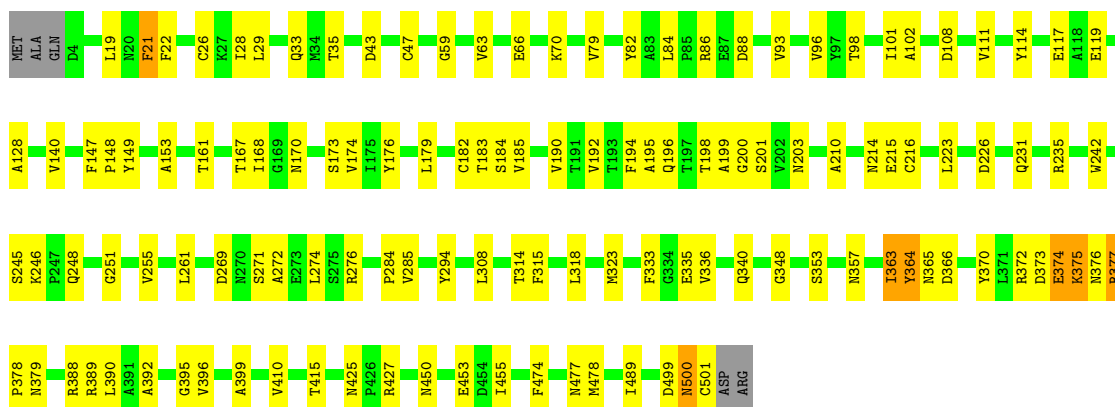
• Molecule 5: Tail sheath protein, gp20

Chain K1: 74% 22%



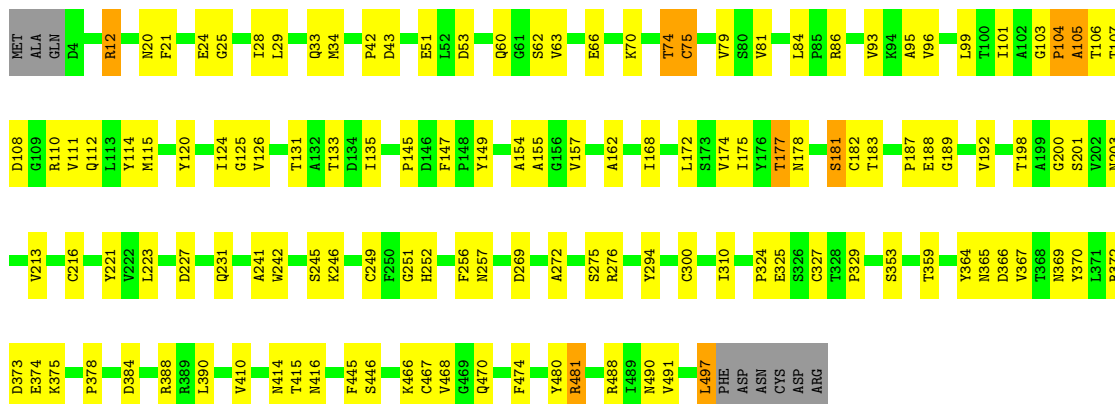
• Molecule 5: Tail sheath protein, gp20

Chain k1: 74% 24% ..



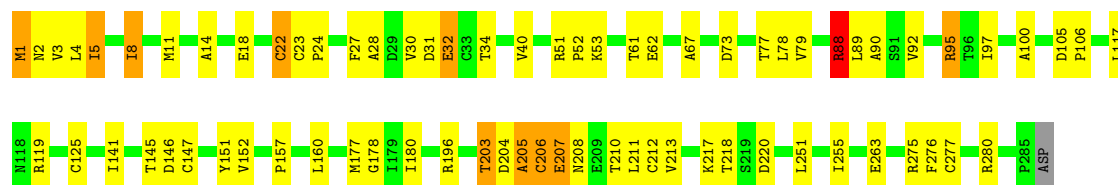
• Molecule 5: Tail sheath protein, gp20

Chain m1: 72% 24% ..



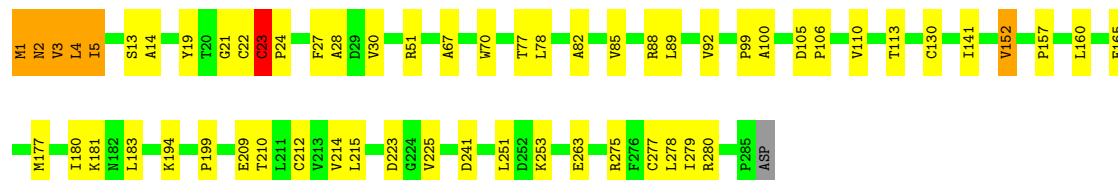
• Molecule 6: Baseplate Wedge 3 protein, gp30

Chain J1: 74% 22% .



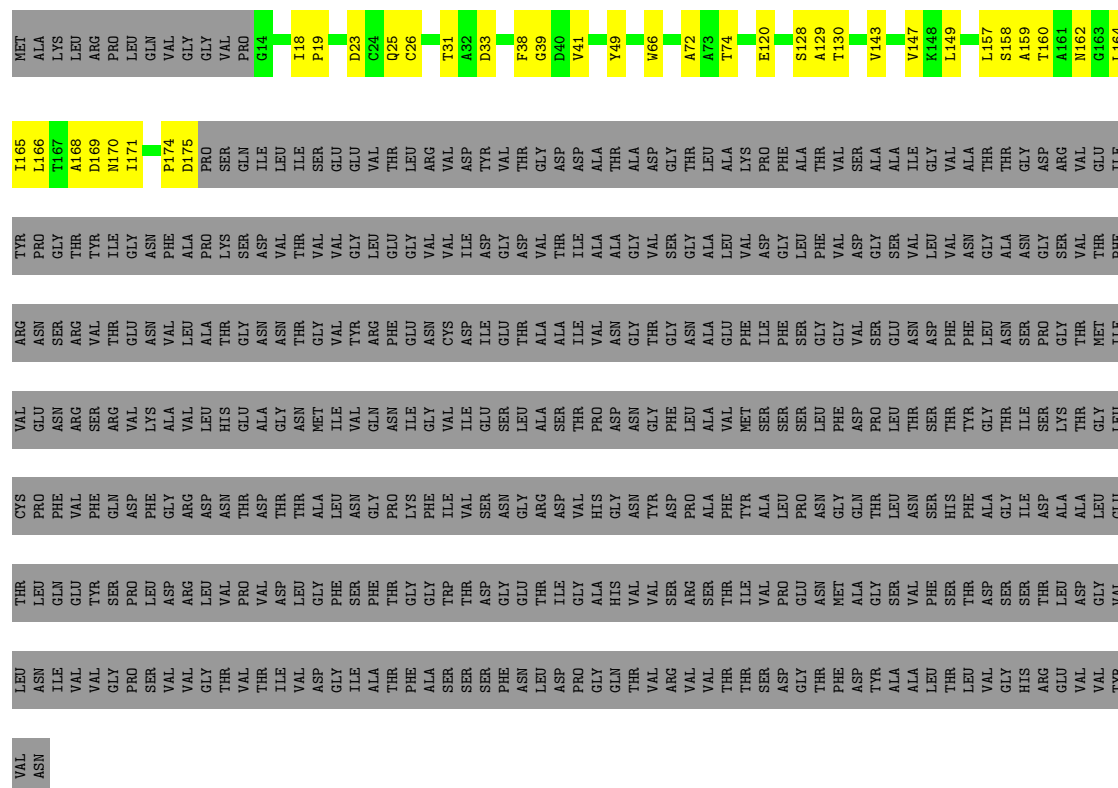
• Molecule 6: Baseplate Wedge 3 protein, gp30

Chain 11: 79% 18%



• Molecule 7: Tail Spike protein, gp124

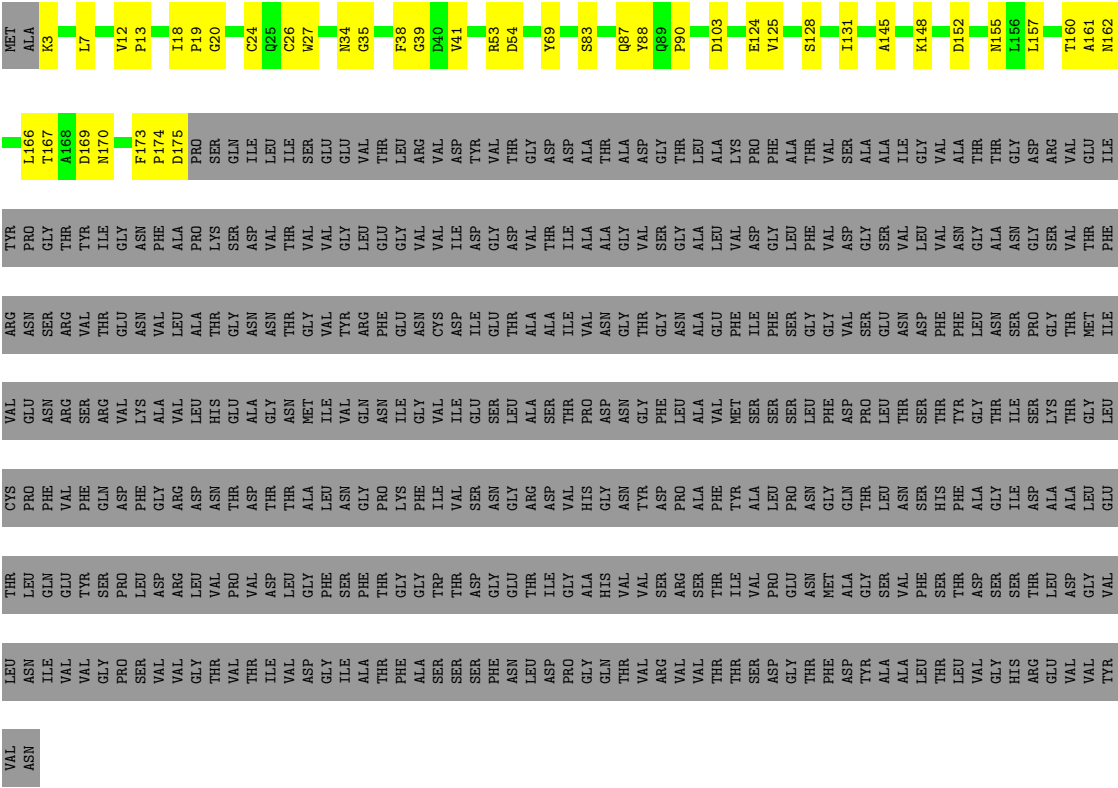
Chain P1: 22% 6% 72%



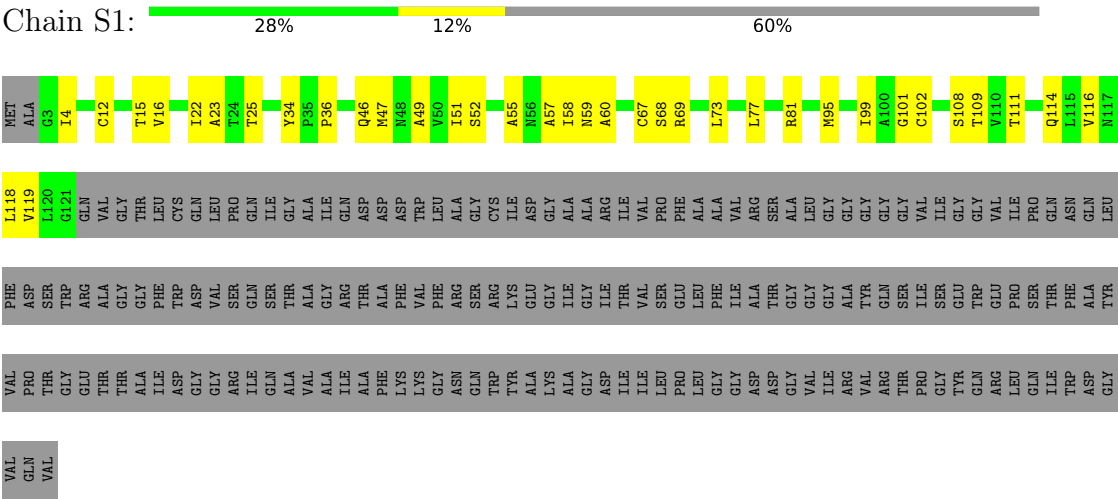
• Molecule 7: Tail Spike protein, gp124

Chain Q1: 23% 6% 71%

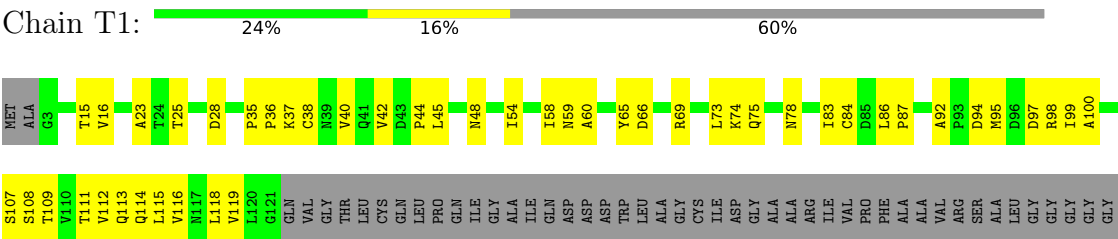




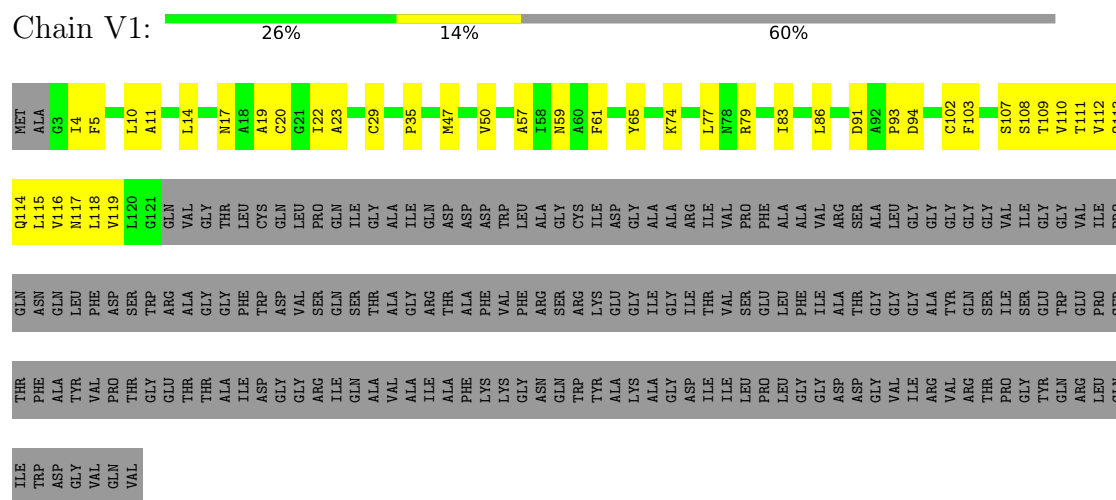
• Molecule 8: Short Tail Fibers, gp31



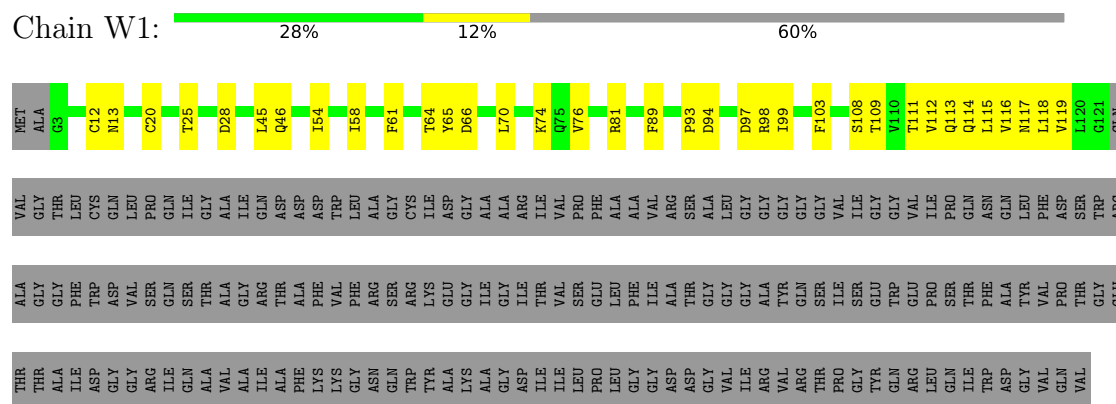
• Molecule 8: Short Tail Fibers, gp31



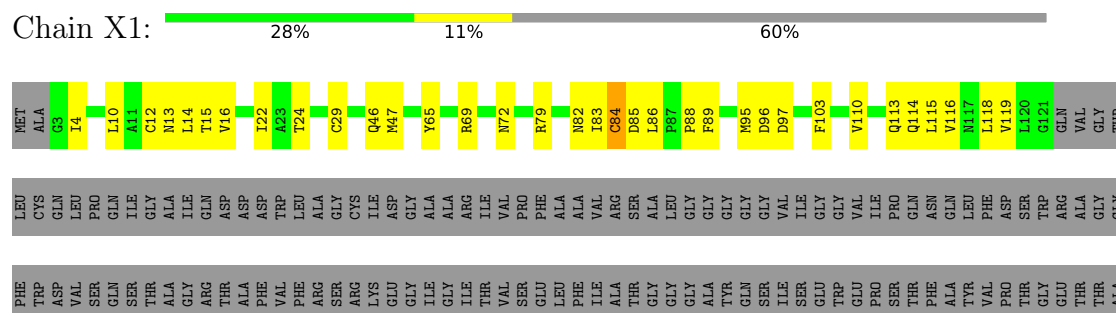
- Molecule 8: Short Tail Fibers, gp31



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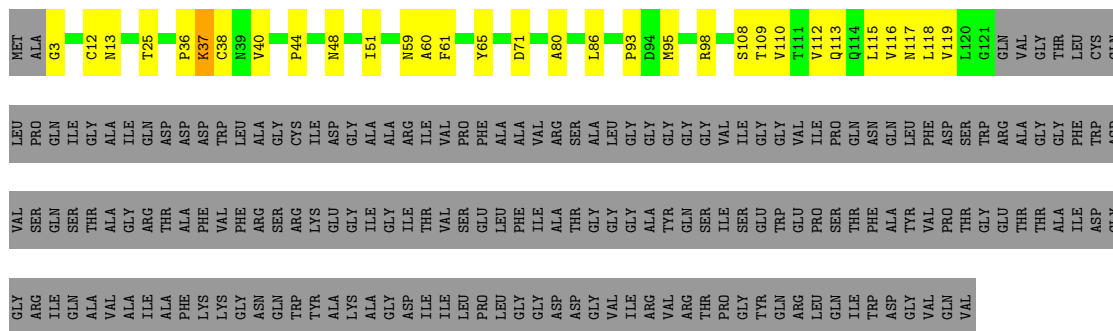


ARG	GLU	VAL	V110	MET
LEU	PRO	ILE	T111	ALA
GLN	SER	PRO	V112	G13
ILE	THR	GLN	Q113	T4
TRP	PHE	ASN	Q114	F5
ASP	ALA	GLN	L115	
GLY	TYR	LEU	V116	G9
VAL	VAL	PHE		L10
GLN	PRO	ASP	V119	A11
VAL	THR	SER	L120	G12
	GLY	TRP	G121	N13
	GLU	ARG	GLN	L14
	THR	ALA	VAL	T15
	THR	GLY	GLY	V16
	ALA	GLY	THR	N17
	ILE	PHE	LEU	
	ASP	TRP	CYS	T22
	GLY	ASP	GLN	A23
	GLY	VAL	LEU	T24
	ARG	SER	PRO	T25
	ILE	GLN	GLN	
	GLN	SER	ILE	C29
	ALA	THR	GLY	
	VAL	ALA	ALA	L32
	ALA	GLY	ILE	Y33
	ILE	ARG	GLN	Y34
	ALA	THR	ASP	
	PHE	ALA	ASP	N47
	LYS	PHE	ASP	N48
	LYS	VAL	TRP	
	GLY	PHE	LEU	F61
	ASN	ARG	ALA	
	GLN	SER	GLY	Y65
	TRP	ARG	CYS	D66
	TYR	LYS	ILE	C67
	ALA	GLU	ASP	S68
	LYS	GLY	GLY	R69
	ALA	ILE	ALA	
	GLY	GLY	ALA	Q75
	ASP	ILE	ARG	
	ILE	THR	ILE	R79
	ILE	VAL	VAL	
	LEU	SER	PRO	T83
	PRO	GLU	PHE	
	LEU	LEU	ALA	L86
	GLY	PHE	ALA	P87
	GLY	ILE	VAL	P88
	ASP	ALA	ARG	
	ASP	THR	SER	P83
	GLY	GLY	ALA	D94
	VAL	GLY	LEU	N95
	ILE	GLY	GLY	
	ARG	ALA	GLY	R98
	VAL	TYR	GLY	I99
	ARG	GLN	GLY	
	THR	SER	GLY	C102
	PRO	ILE	VAL	
	GLY	SER	ILE	Q106
	TYR	GLU	GLY	
	GLN	THR	GLY	T102

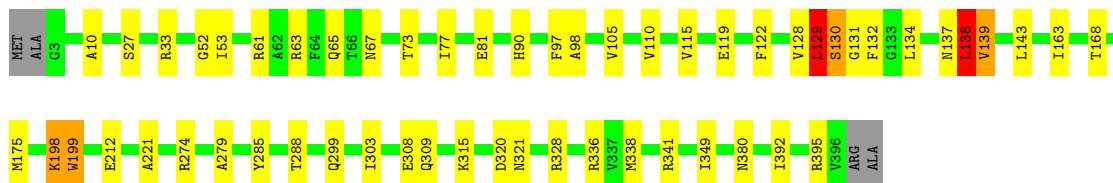
GLY	TYR	LEU	N117	MET
	VAL	ASP	L118	ALA
GLN	PRO	SER	V119	G3
VAL	THR	TRP	L120	
	GLY	ARG	G121	G12
	GLU	ALA	GLN	N13
	THR	GLY	VAL	
	THR	GLY	VAL	I22
	ALA	GLY	THR	A23
	ILE	PHE	LEU	T24
	ASP	TRP	CYS	T25
	GLY	ASP	GLN	
	GLY	VAL	LEU	M47
	ILE	SER	PRO	V50
	GLN	SER	ILE	
	ALA	THR	GLY	I54
	VAL	ALA	ALA	
	ILE	GLY	ILE	I58
	ALA	ARG	GLN	
	ALA	THR	ASP	F61
	PHE	ALA	ASP	
	LYS	PHE	ASP	T64
	LYS	VAL	TRP	Y65
	GLY	PHE	LEU	D86
	ASN	ARG	ALA	C87
	GLN	SER	GLY	S68
	TRP	ARG	CYS	
	TYR	LYS	ILE	D71
	ALA	GLU	ASP	
	LYS	GLY	GLY	K74
	ALA	ILE	ALA	G75
	GLY	GLY	ALA	V76
	ASP	ILE	ARG	L77
	ILE	THR	ILE	
	ILE	VAL	VAL	R81
	LEU	SER	PRO	N82
	PRO	GLU	PHE	I83
	LEU	LEU	ALA	
	GLY	PHE	ALA	P88
	GLY	ILE	VAL	F89
	ASP	ALA	ARG	
	ASP	THR	SER	D94
	GLY	GLY	ALA	M95
	VAL	GLY	LEU	
	ILE	GLY	GLY	R98
	ARG	ALA	GLY	I99
	VAL	THR	GLY	
	ARG	GLN	GLY	C102
	THR	SER	GLY	
	PRO	ILE	VAL	S107
	TYR	SER	ILE	T108
	TYR	GLU	GLY	T109
	GLN	TRP	GLY	V110
	ARG	GLU	VAL	T111
	LEU	PRO	ILE	V112
	GLN	SER	PRO	Q113
	ILE	THR	GLN	Q114
	TRP	PHE	ASN	L115
	ASP	ALA	CYN	H116

VAL	THR	SER	L120	MET
	GLY	TRP	GLN	ALA
	GLU	ARG	VAL	G3
	THR	ALA	GLY	I4
	THR	GLY	THR	S7
	ALA	GLY	THR	G8
	ILE	PHE	LEU	G9
	ASP	PHE	CYS	L10
	GLY	ASP	GLN	
	GLY	VAL	LEU	L14
	ARG	SER	PRO	T15
	ILE	GLN	GLN	V16
	GLN	SER	ILE	
	ALA	THR	GLY	I22
	VAL	ALA	ALA	
	ALA	GLY	ILE	T25
	ILE	ARG	GLN	
	ALA	THR	ASP	L32
	PHE	ALA	ASP	
	LYS	PHE	ASP	V40
	LYS	VAL	TRP	
	GLY	PHE	LEU	Q46
	ASN	ARG	ALA	
	GLN	SER	GLY	N59
	TRP	ARG	CYS	
	TYR	LYS	ILE	Y65
	ALA	GLU	ASP	D66
	LYS	GLY	GLY	
	ALA	ILE	ALA	R69
	GLY	GLY	ALA	
	ASP	ILE	ARG	N72
	ILE	THR	ILE	
	ILE	VAL	VAL	C84
	LEU	SER	PRO	
	PRO	GLU	PHE	D85
	LEU	LEU	ALA	L86
	GLY	PHE	ALA	P87
	GLY	ILE	VAL	P88
	ASP	ILE	VAL	F89
	ASP	ALA	ARG	G90
	ASP	THR	SER	D91
	GLY	GLY	ALA	A92
	VAL	GLY	LEU	
	ILE	GLY	GLY	F93
	ARG	ALA	GLY	D94
	VAL	TYR	GLY	N95
	ARG	GLN	GLY	
	THR	SER	GLY	R98
	PRO	ILE	VAL	
	GLY	SER	ILE	S107
	TYR	GLU	GLY	T108
	GLN	TRP	GLY	S109
	LEU	GLU	VAL	
	ARG	PRO	ILE	V112
	GLN	SER	PRO	Q113
	ILE	THR	GLN	Q114
	TRP	PHE	ASN	L115
	ASP	ALA	GLN	V116
	GLY	TYR	LEU	N117
	VAL	VAL	PHE	L118
	GLN	PRO	ASP	V119

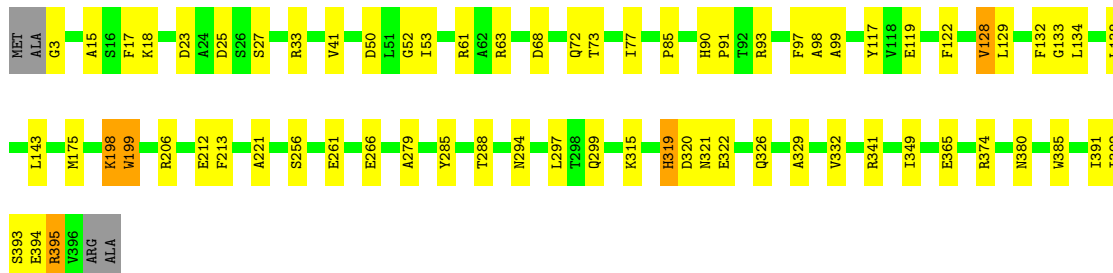
Chain z1: 29% 10% 60%



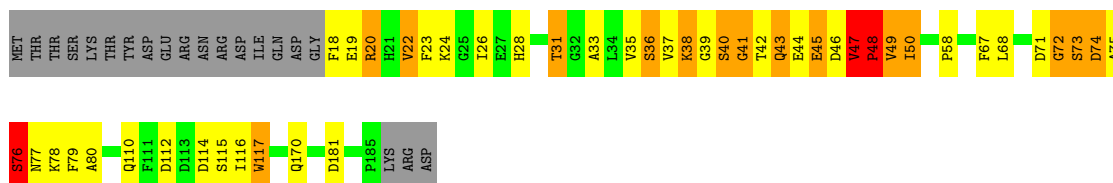
Chain U1: 85% 13% ..



Chain e1: 81% 16%



Chain A: 64% 15% 8% 1% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14856	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.478	Depositor
Minimum map value	-0.780	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	624.24005, 624.24005, 624.24005	wwPDB
Map dimensions	578, 578, 578	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	C1	0.42	1/2598 (0.0%)	0.61	3/3525 (0.1%)
2	E1	0.43	0/1011	0.46	0/1382
2	a1	0.32	0/1011	0.46	1/1382 (0.1%)
2	f1	0.31	0/1011	0.39	0/1382
2	g1	0.33	0/1011	0.43	0/1382
3	F1	0.40	0/3085	0.47	1/4207 (0.0%)
3	G1	0.50	1/3085 (0.0%)	0.62	5/4207 (0.1%)
3	h1	0.41	0/3085	0.48	1/4207 (0.0%)
3	i1	0.51	0/3085	0.56	0/4207
4	H1	0.34	0/1353	0.47	0/1831
4	j1	0.30	0/1353	0.48	0/1831
5	I1	0.40	0/3815	0.50	3/5211 (0.1%)
5	K1	0.38	1/3781 (0.0%)	0.53	3/5165 (0.1%)
5	k1	0.38	0/3815	0.50	1/5211 (0.0%)
5	m1	0.34	0/3781	0.50	0/5165
6	J1	0.50	1/2237 (0.0%)	0.56	2/3063 (0.1%)
6	l1	0.43	0/2237	0.52	0/3063
7	P1	0.21	0/1269	0.36	0/1755
7	Q1	0.29	0/1352	0.46	0/1868
7	R1	0.19	0/1352	0.38	1/1868 (0.1%)
7	r1	0.22	0/1269	0.37	0/1755
7	s1	0.28	0/1352	0.43	0/1868
7	t1	0.20	0/1352	0.39	0/1868
8	S1	0.16	0/892	0.35	0/1217
8	T1	0.17	0/892	0.38	0/1217
8	V1	0.17	0/892	0.41	0/1217
8	W1	0.23	0/892	0.37	0/1217
8	X1	0.22	0/892	0.40	0/1217
8	Y1	0.19	0/892	0.36	0/1217
8	u1	0.20	0/892	0.41	0/1217
8	v1	0.21	0/892	0.38	0/1217
8	w1	0.16	0/892	0.36	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	x1	0.16	0/892	0.36	0/1217
8	y1	0.21	0/892	0.38	0/1217
8	z1	0.23	0/892	0.39	0/1217
9	U1	0.40	0/3093	0.50	4/4214 (0.1%)
9	e1	0.41	0/3093	0.47	1/4214 (0.0%)
10	A	0.81	0/1320	1.28	13/1791 (0.7%)
All	All	0.38	4/67510 (0.0%)	0.51	39/92226 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G1	188	TYR	CA-C	-7.62	1.45	1.52
6	J1	88	ARG	CA-C	-5.74	1.45	1.52
1	C1	59	VAL	CA-C	-5.62	1.48	1.53
5	K1	357	ASN	CA-C	-5.06	1.50	1.53

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	73	SER	N-CA-C	-10.78	97.64	112.30
10	A	39	GLY	N-CA-C	-10.73	101.79	115.42
10	A	44	GLU	N-CA-C	-9.42	101.04	112.54
3	h1	336	ILE	N-CA-C	-8.12	101.07	113.16
3	G1	187	ARG	N-CA-C	-8.01	101.33	113.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	2551	0	2522	127	0
2	E1	995	0	968	10	0
2	a1	995	0	968	19	0
2	f1	995	0	969	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	g1	995	0	968	13	0
3	F1	3016	0	2903	47	0
3	G1	3016	0	2901	66	0
3	h1	3016	0	2902	36	0
3	i1	3016	0	2905	58	0
4	H1	1334	0	1308	30	0
4	j1	1334	0	1307	30	0
5	I1	3739	0	3607	84	0
5	K1	3706	0	3585	84	0
5	k1	3739	0	3606	85	0
5	m1	3706	0	3586	91	0
6	J1	2185	0	2140	53	0
6	l1	2185	0	2140	46	0
7	P1	1227	0	1119	33	0
7	Q1	1308	0	1213	31	0
7	R1	1308	0	1214	42	0
7	r1	1227	0	1118	31	0
7	s1	1308	0	1212	29	0
7	t1	1308	0	1212	33	0
8	S1	878	0	844	41	0
8	T1	878	0	844	50	0
8	V1	878	0	844	37	0
8	W1	878	0	844	36	0
8	X1	878	0	845	29	0
8	Y1	878	0	845	31	0
8	u1	878	0	844	31	0
8	v1	878	0	845	51	0
8	w1	878	0	844	34	0
8	x1	878	0	844	44	0
8	y1	878	0	844	39	0
8	z1	878	0	844	29	0
9	U1	3027	0	2908	46	0
9	e1	3027	0	2906	59	0
10	A	1289	0	1201	55	0
11	A	1	0	0	0	0
All	All	66089	0	63519	1421	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1421 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)
3:G1:269:PRO:HD2	3:G1:274:LEU:HD12	1.36	1.04
7:R1:24:CYS:SG	7:R1:24:CYS:O	2.16	1.04
3:G1:68:CYS:O	3:G1:68:CYS:SG	2.16	1.04
6:l1:5:ILE:HD11	6:l1:14:ALA:HB2	1.43	0.99
3:G1:268:SER:HB2	3:G1:269:PRO:HD3	1.46	0.96

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	C1	320/457 (70%)	247 (77%)	65 (20%)	8 (2%)	4	27
2	E1	129/136 (95%)	117 (91%)	12 (9%)	0	100	100
2	a1	129/136 (95%)	117 (91%)	12 (9%)	0	100	100
2	f1	129/136 (95%)	118 (92%)	11 (8%)	0	100	100
2	g1	129/136 (95%)	118 (92%)	10 (8%)	1 (1%)	16	50
3	F1	391/396 (99%)	371 (95%)	19 (5%)	1 (0%)	36	68
3	G1	391/396 (99%)	366 (94%)	21 (5%)	4 (1%)	12	45
3	h1	391/396 (99%)	378 (97%)	10 (3%)	3 (1%)	16	50
3	i1	391/396 (99%)	363 (93%)	26 (7%)	2 (0%)	24	59
4	H1	174/178 (98%)	149 (86%)	24 (14%)	1 (1%)	21	56
4	j1	174/178 (98%)	145 (83%)	27 (16%)	2 (1%)	11	43
5	I1	496/503 (99%)	439 (88%)	56 (11%)	1 (0%)	43	73
5	K1	492/503 (98%)	421 (86%)	64 (13%)	7 (1%)	9	39
5	k1	496/503 (99%)	441 (89%)	53 (11%)	2 (0%)	30	62
5	m1	492/503 (98%)	404 (82%)	80 (16%)	8 (2%)	7	36
6	J1	283/286 (99%)	258 (91%)	20 (7%)	5 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	l1	283/286 (99%)	253 (89%)	27 (10%)	3 (1%)	11	43
7	P1	160/587 (27%)	146 (91%)	13 (8%)	1 (1%)	21	56
7	Q1	171/587 (29%)	155 (91%)	12 (7%)	4 (2%)	5	29
7	R1	171/587 (29%)	158 (92%)	12 (7%)	1 (1%)	21	56
7	r1	160/587 (27%)	147 (92%)	12 (8%)	1 (1%)	21	56
7	s1	171/587 (29%)	158 (92%)	10 (6%)	3 (2%)	6	34
7	t1	171/587 (29%)	156 (91%)	15 (9%)	0	100	100
8	S1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	T1	117/300 (39%)	112 (96%)	4 (3%)	1 (1%)	14	47
8	V1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	W1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	X1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	Y1	117/300 (39%)	111 (95%)	6 (5%)	0	100	100
8	u1	117/300 (39%)	110 (94%)	6 (5%)	1 (1%)	14	47
8	v1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	w1	117/300 (39%)	114 (97%)	3 (3%)	0	100	100
8	x1	117/300 (39%)	105 (90%)	12 (10%)	0	100	100
8	y1	117/300 (39%)	110 (94%)	7 (6%)	0	100	100
8	z1	117/300 (39%)	108 (92%)	7 (6%)	2 (2%)	7	35
9	U1	392/398 (98%)	368 (94%)	21 (5%)	3 (1%)	16	50
9	e1	392/398 (98%)	361 (92%)	30 (8%)	1 (0%)	36	68
10	A	166/188 (88%)	142 (86%)	13 (8%)	11 (7%)	1	7
All	All	8648/13631 (63%)	7807 (90%)	764 (9%)	77 (1%)	16	47

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F1	375	ASP
6	J1	2	ASN
5	K1	378	PRO
7	Q1	117	ILE
7	Q1	119	VAL

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	C1	281/383 (73%)	270 (96%)	11 (4%)	28	62
2	E1	115/116 (99%)	115 (100%)	0	100	100
2	a1	115/116 (99%)	115 (100%)	0	100	100
2	f1	115/116 (99%)	115 (100%)	0	100	100
2	g1	115/116 (99%)	115 (100%)	0	100	100
3	F1	330/333 (99%)	325 (98%)	5 (2%)	57	76
3	G1	330/333 (99%)	315 (96%)	15 (4%)	24	58
3	h1	330/333 (99%)	325 (98%)	5 (2%)	57	76
3	i1	330/333 (99%)	323 (98%)	7 (2%)	47	71
4	H1	145/147 (99%)	145 (100%)	0	100	100
4	j1	145/147 (99%)	145 (100%)	0	100	100
5	I1	404/408 (99%)	400 (99%)	4 (1%)	68	80
5	K1	400/408 (98%)	392 (98%)	8 (2%)	48	72
5	k1	404/408 (99%)	394 (98%)	10 (2%)	42	69
5	m1	400/408 (98%)	392 (98%)	8 (2%)	48	72
6	J1	245/247 (99%)	228 (93%)	17 (7%)	14	45
6	l1	245/247 (99%)	239 (98%)	6 (2%)	43	70
7	P1	129/473 (27%)	128 (99%)	1 (1%)	73	82
7	Q1	138/473 (29%)	136 (99%)	2 (1%)	59	77
7	R1	138/473 (29%)	135 (98%)	3 (2%)	45	71
7	r1	129/473 (27%)	127 (98%)	2 (2%)	55	75
7	s1	138/473 (29%)	135 (98%)	3 (2%)	45	71
7	t1	138/473 (29%)	137 (99%)	1 (1%)	76	83
8	S1	97/229 (42%)	96 (99%)	1 (1%)	68	80
8	T1	97/229 (42%)	97 (100%)	0	100	100
8	V1	97/229 (42%)	96 (99%)	1 (1%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	W1	97/229 (42%)	97 (100%)	0	100	100
8	X1	97/229 (42%)	96 (99%)	1 (1%)	68	80
8	Y1	97/229 (42%)	97 (100%)	0	100	100
8	u1	97/229 (42%)	95 (98%)	2 (2%)	47	71
8	v1	97/229 (42%)	95 (98%)	2 (2%)	47	71
8	w1	97/229 (42%)	97 (100%)	0	100	100
8	x1	97/229 (42%)	97 (100%)	0	100	100
8	y1	97/229 (42%)	97 (100%)	0	100	100
8	z1	97/229 (42%)	94 (97%)	3 (3%)	35	66
9	U1	314/316 (99%)	307 (98%)	7 (2%)	45	71
9	e1	314/316 (99%)	308 (98%)	6 (2%)	50	73
10	A	143/162 (88%)	133 (93%)	10 (7%)	14	45
All	All	7194/10979 (66%)	7053 (98%)	141 (2%)	48	72

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	m1	481	ARG
7	r1	175	ASP
8	z1	40	VAL
6	J1	212	CYS
6	J1	211	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
7	t1	94	ASN
8	v1	113	GLN
8	y1	117	ASN
7	Q1	82	ASN
7	P1	25	GLN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

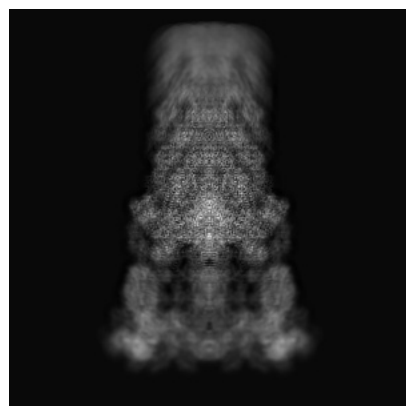
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29383. These allow visual inspection of the internal detail of the map and identification of artifacts.

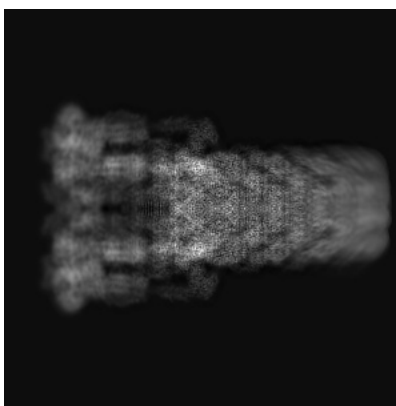
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

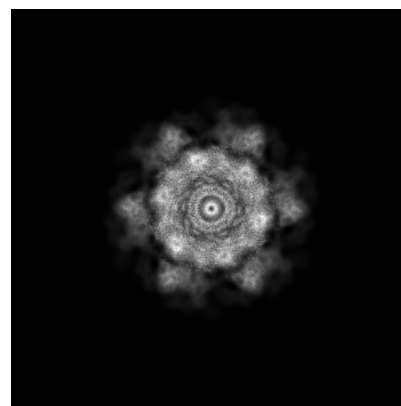
6.1.1 Primary map



X

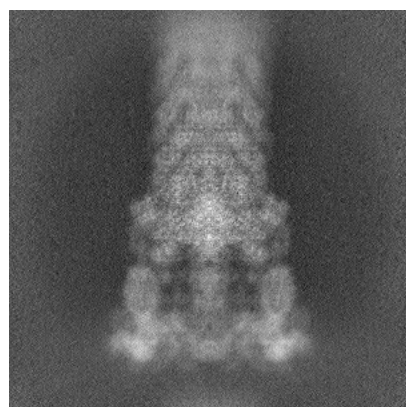


Y

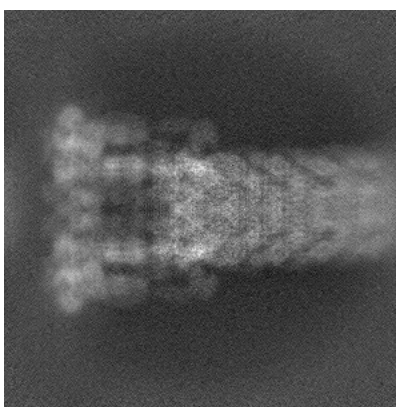


Z

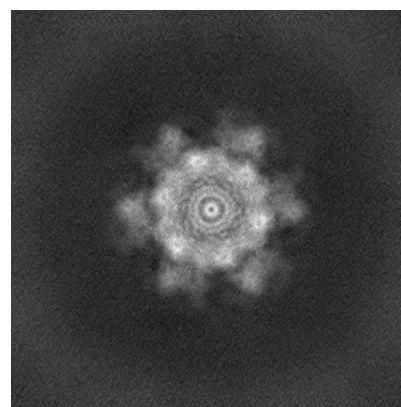
6.1.2 Raw map



X



Y

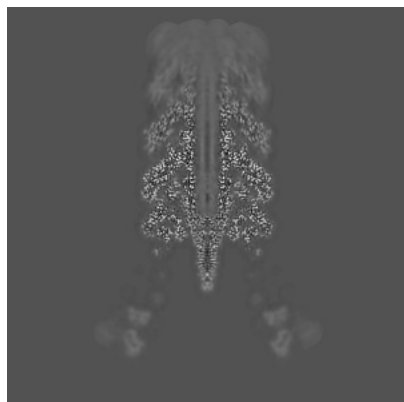


Z

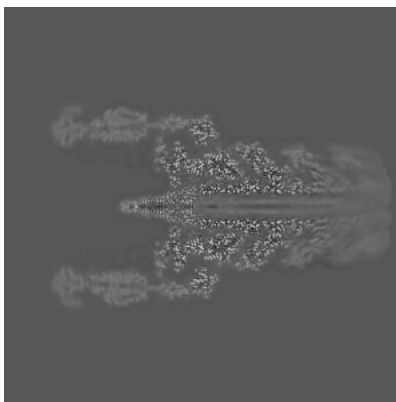
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

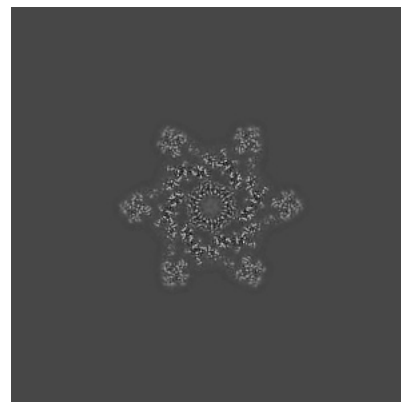
6.2.1 Primary map



X Index: 289

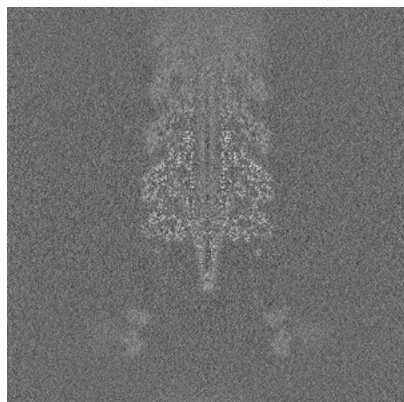


Y Index: 289

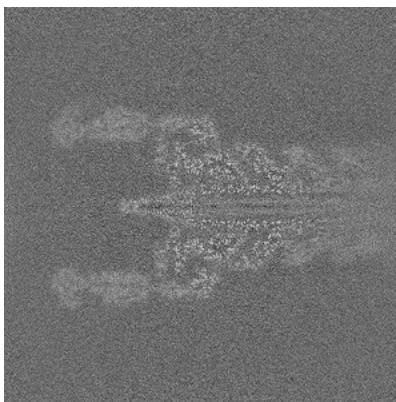


Z Index: 289

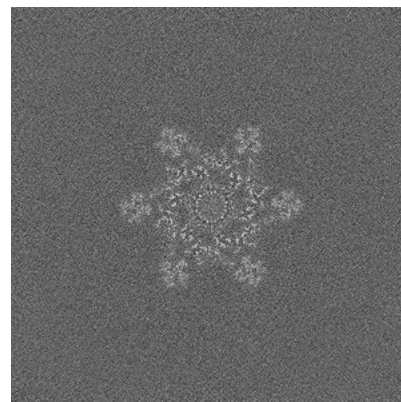
6.2.2 Raw map



X Index: 289



Y Index: 289

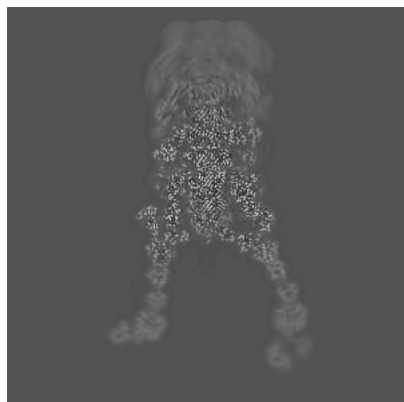


Z Index: 289

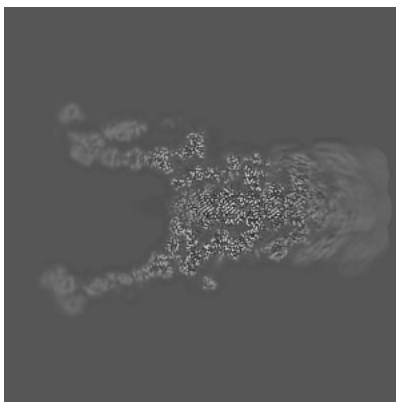
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

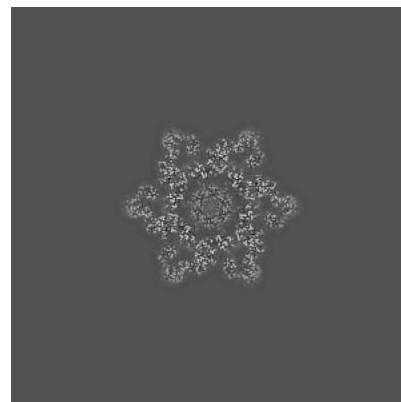
6.3.1 Primary map



X Index: 310

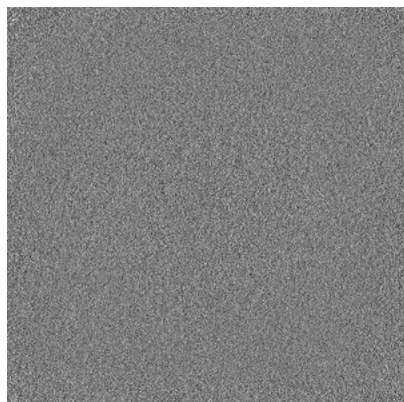


Y Index: 268

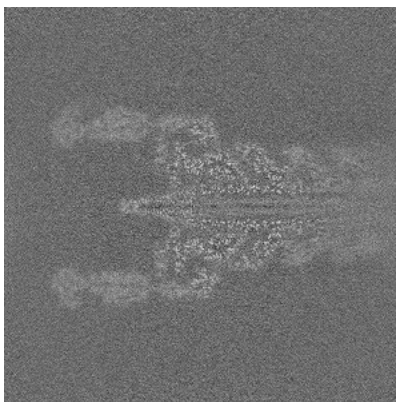


Z Index: 276

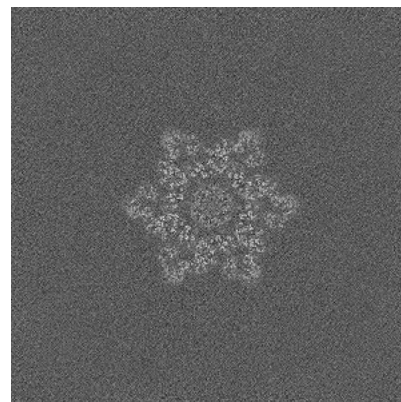
6.3.2 Raw map



X Index: 0



Y Index: 289

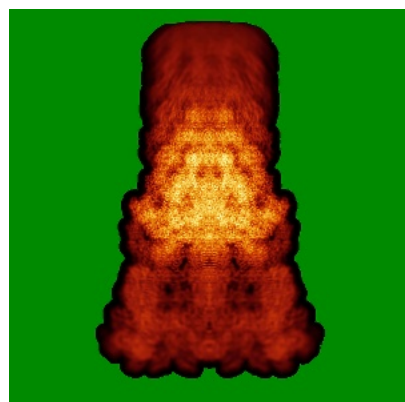


Z Index: 276

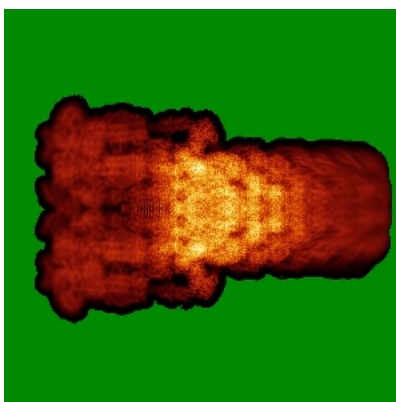
The images above show the largest variance slices of the map in three orthogonal directions.

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

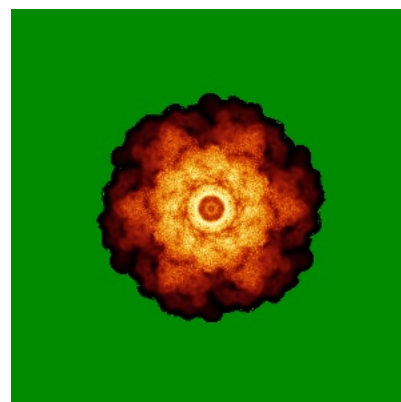
6.4.1 Primary map



X

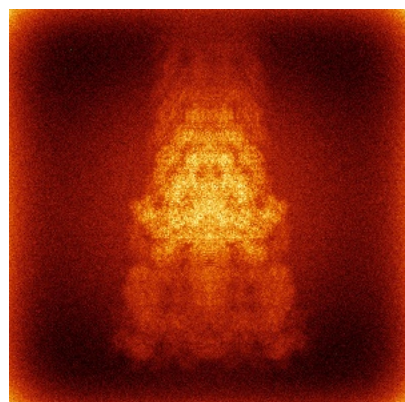


Y

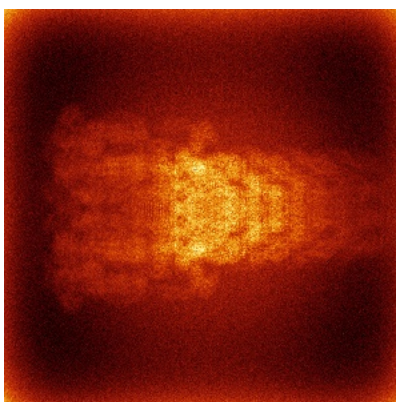


Z

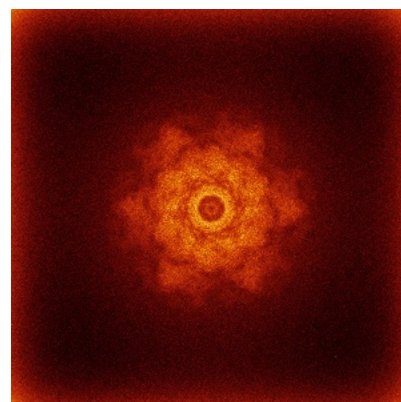
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

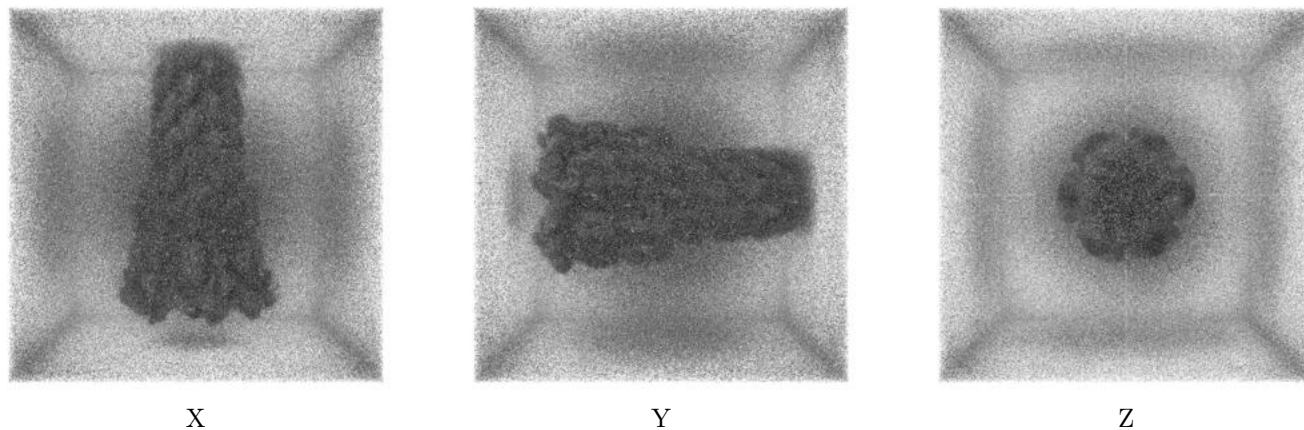
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

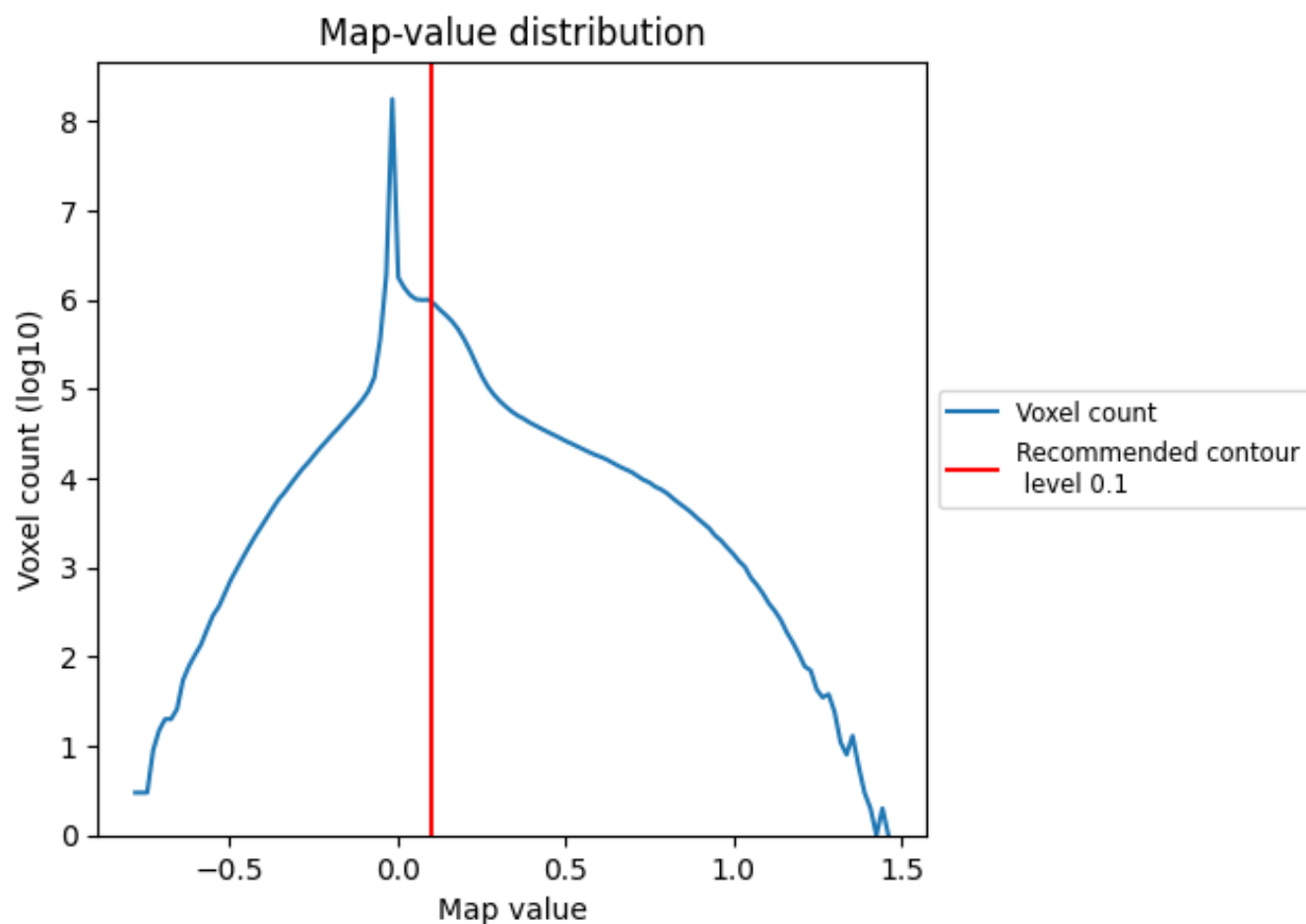
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

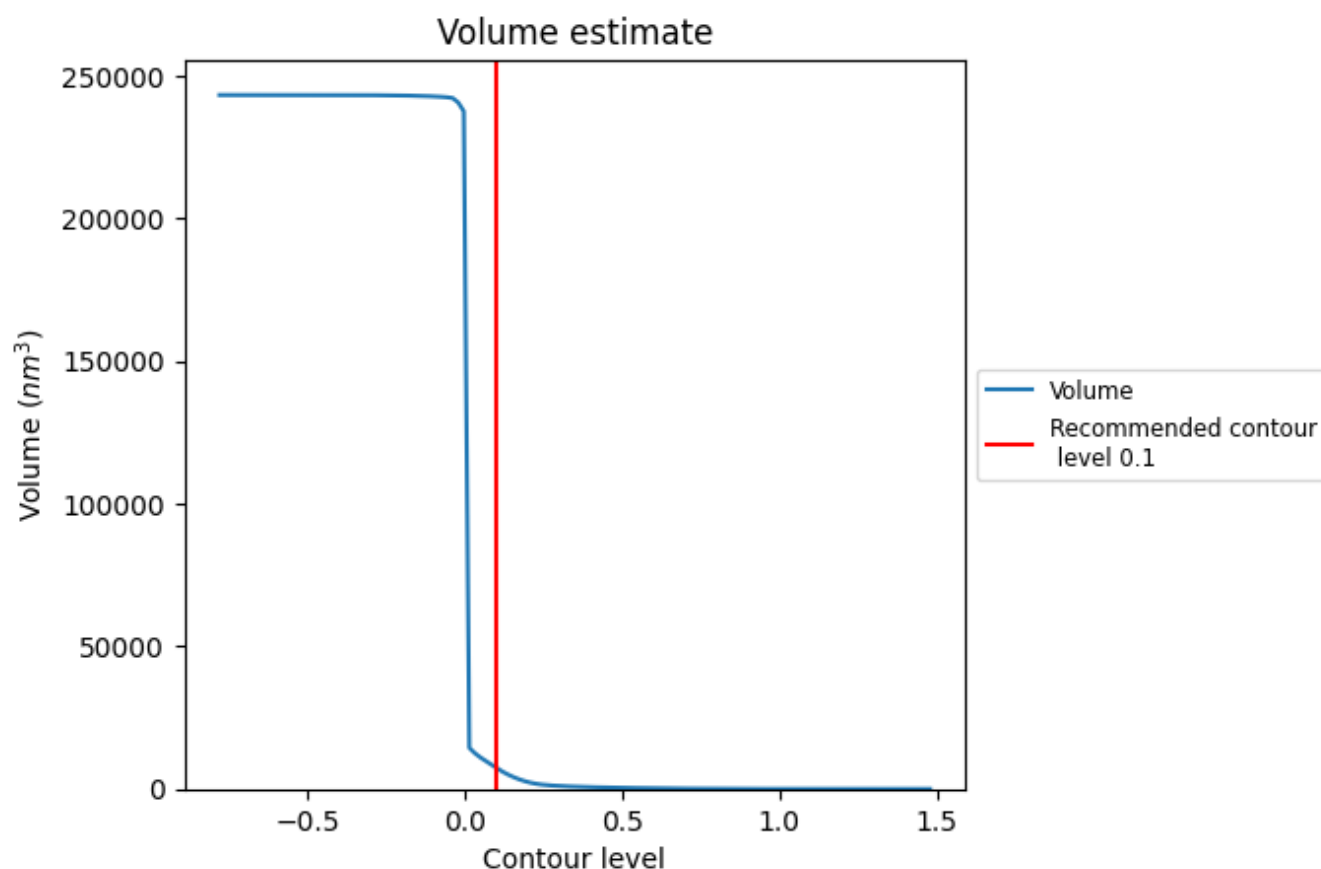
This section contains the results of statistical analysis of the map.

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.

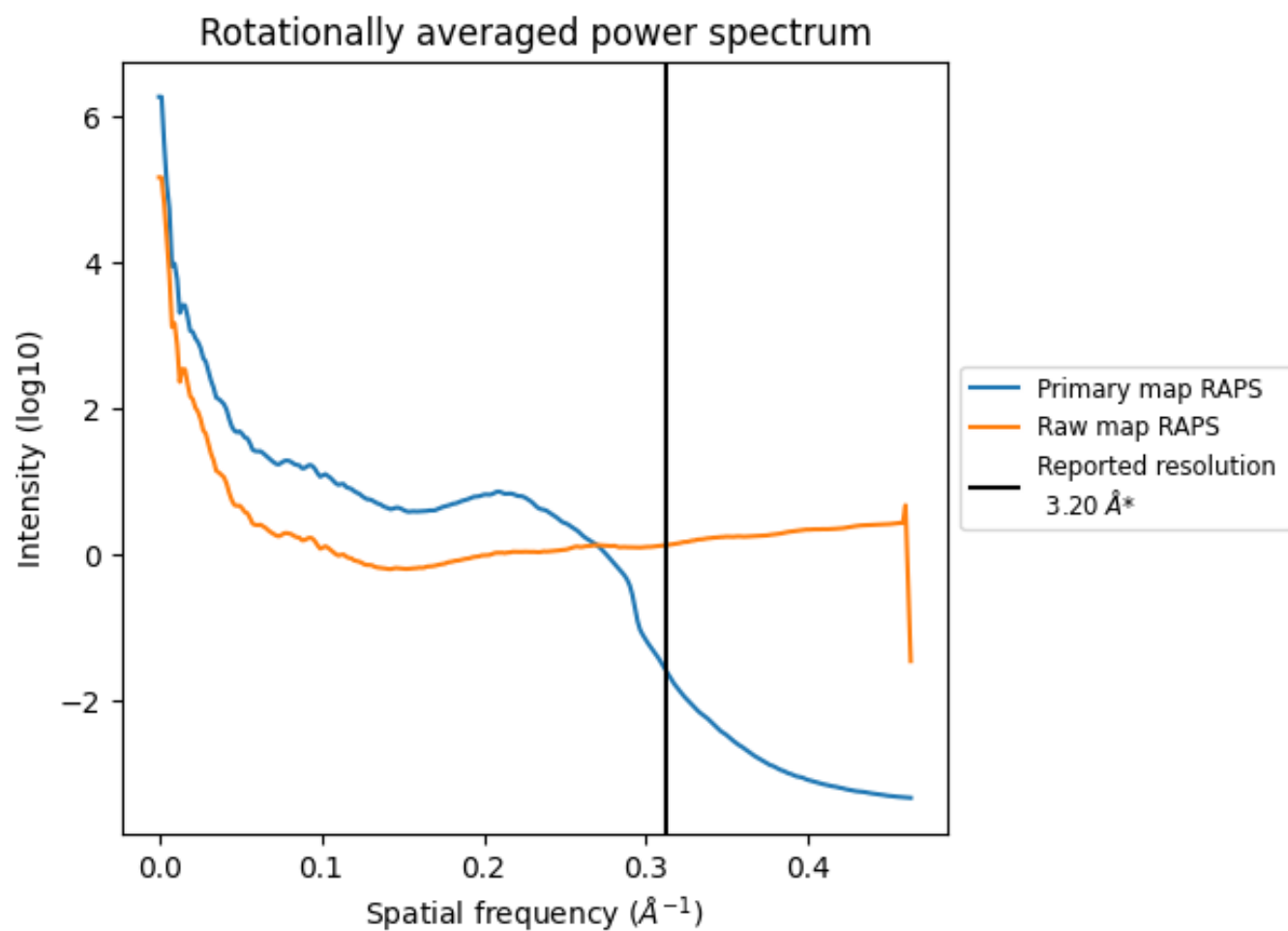
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7391 nm^3 ; this corresponds to an approximate mass of 6676 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 ⓘ

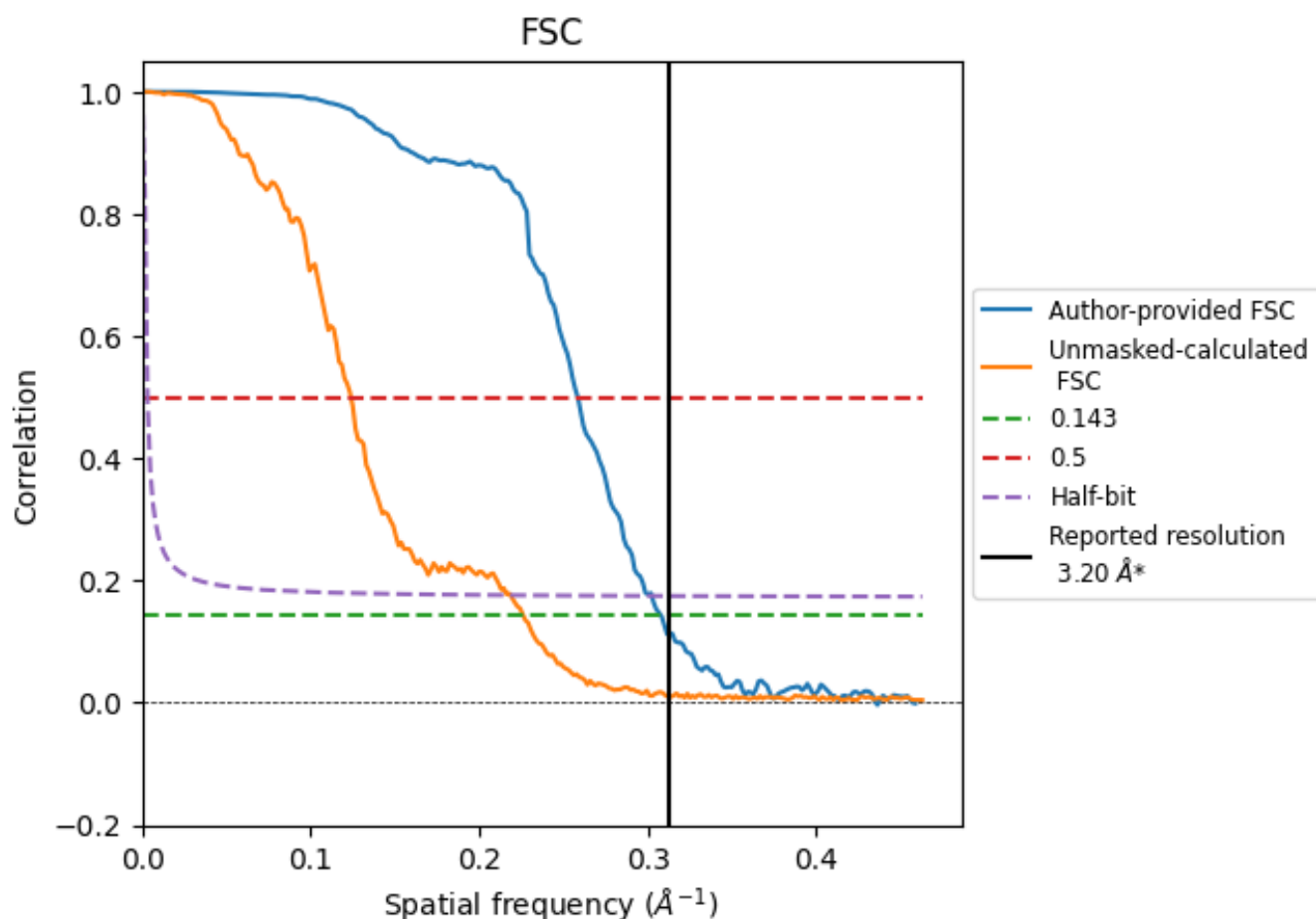


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.25	3.87	3.31
Unmasked-calculated*	4.42	8.07	4.58

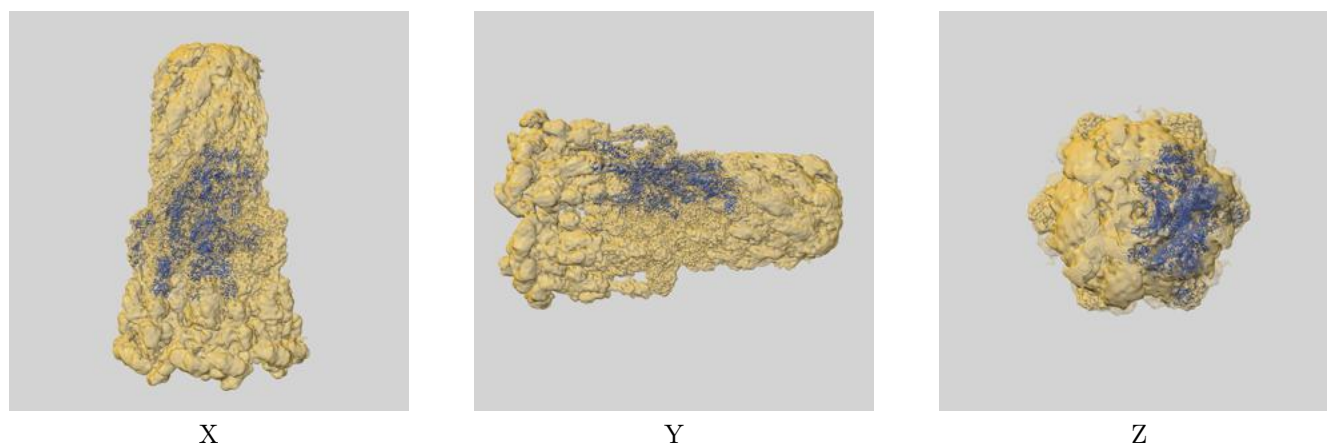
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

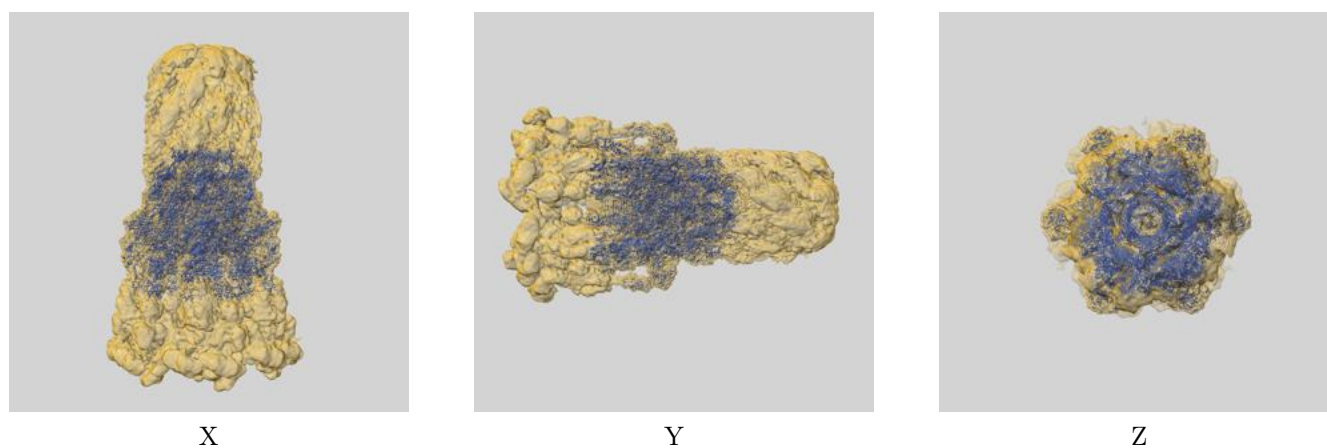
This section contains information regarding the fit between EMDB map EMD-29383 and PDB model 8FQC. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

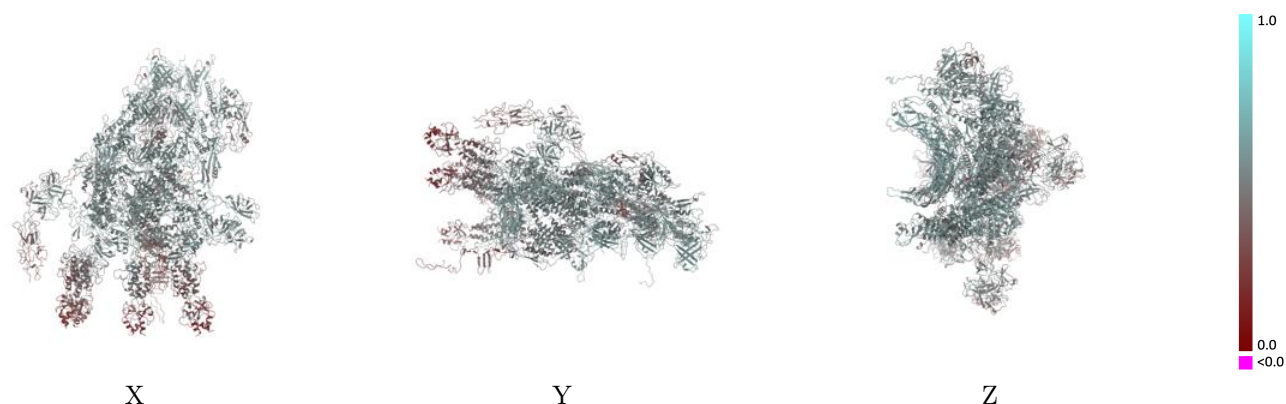


9.1.2 Map-model assembly overlay [i](#)



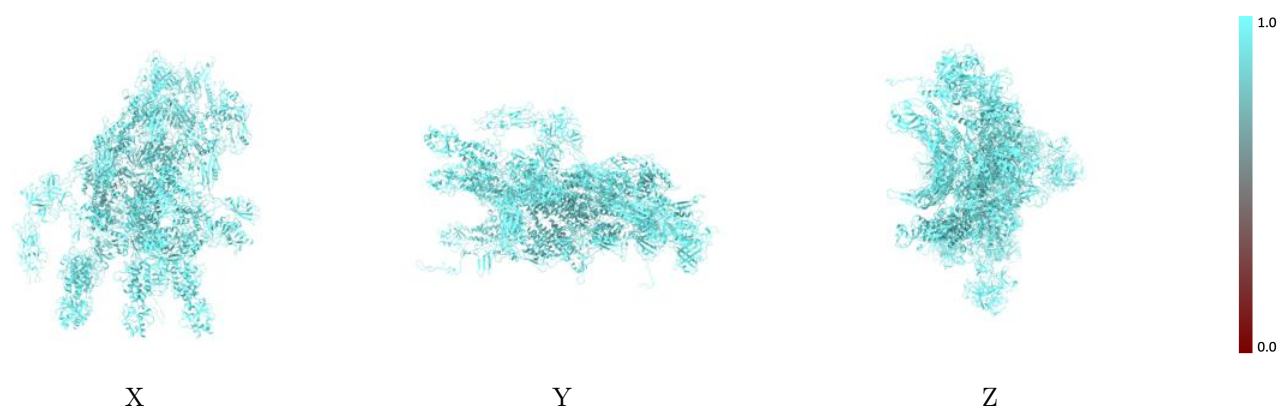
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



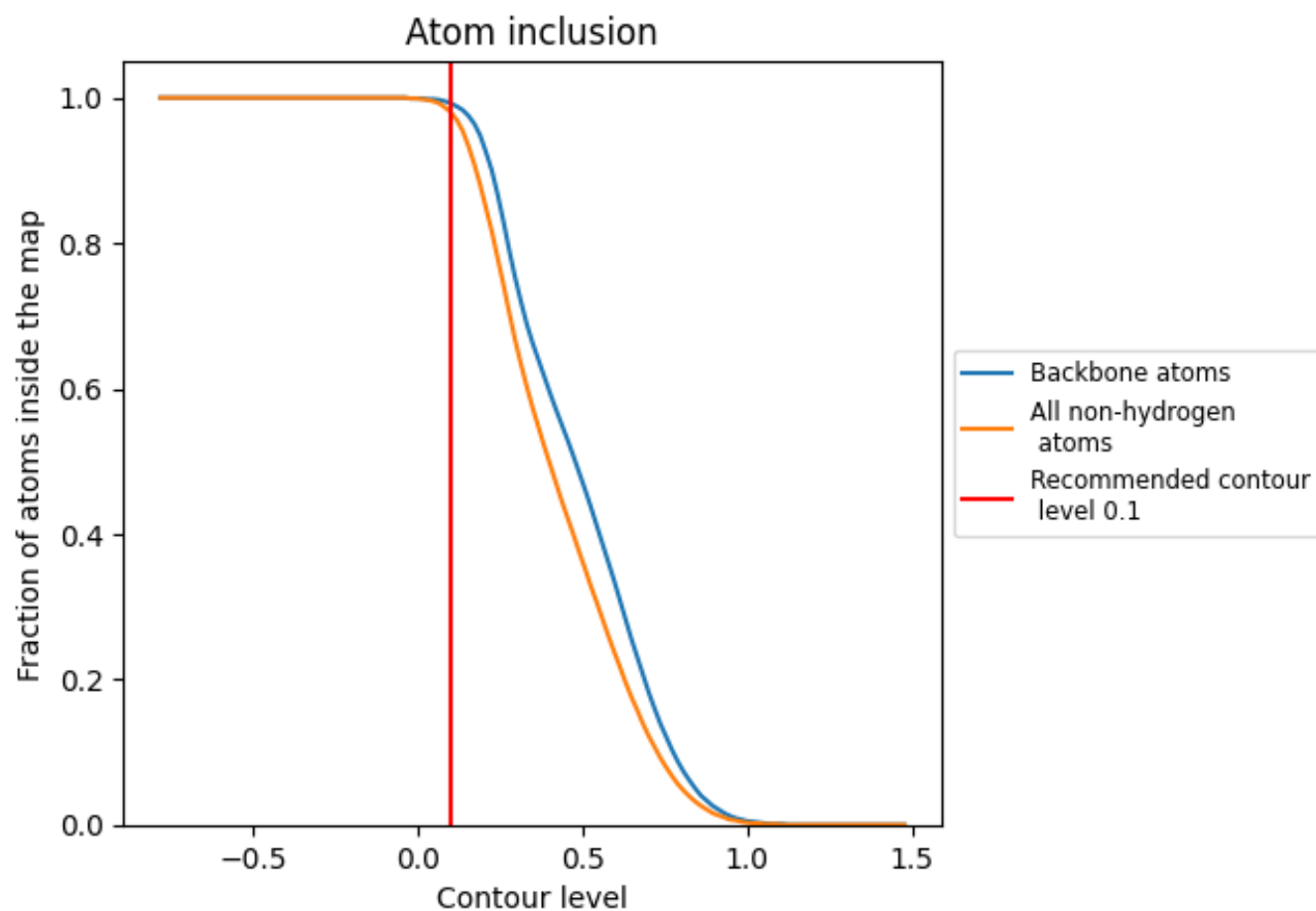
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.4980
A	 0.9070	 0.3820
C1	 0.9400	 0.4770
E1	 0.9870	 0.5640
F1	 0.9840	 0.5370
G1	 0.9880	 0.5390
H1	 0.9770	 0.5290
I1	 0.9860	 0.5410
J1	 0.9880	 0.5400
K1	 0.9790	 0.4980
P1	 0.9880	 0.4520
Q1	 0.9890	 0.4560
R1	 0.9820	 0.4260
S1	 0.9780	 0.3790
T1	 0.9900	 0.3780
U1	 0.9780	 0.5470
V1	 0.9820	 0.3670
W1	 0.9910	 0.4300
X1	 0.9860	 0.4260
Y1	 0.9900	 0.4110
a1	 0.9840	 0.5560
e1	 0.9790	 0.5530
f1	 0.9910	 0.5590
g1	 0.9820	 0.5630
h1	 0.9840	 0.5390
i1	 0.9860	 0.5380
j1	 0.9780	 0.5300
k1	 0.9890	 0.5440
l1	 0.9840	 0.5380
m1	 0.9800	 0.5010
r1	 0.9860	 0.4470
s1	 0.9890	 0.4560
t1	 0.9870	 0.4320
u1	 0.9830	 0.4140
v1	 0.9760	 0.3780



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Chain	Atom inclusion	Q-score
w1	 0.9820	 0.3860
x1	 0.9680	 0.3610
y1	 0.9850	 0.4160
z1	 0.9780	 0.4070