



Full wwPDB EM Validation Report ⓘ

Apr 4, 2024 – 11:10 AM JST

PDB ID : 8XPM
EMDB ID : EMD-38556
Title : Mature virion portal of phage lambda with DNA
Authors : Wang, J.W.; Gu, Z.W.
Deposited on : 2024-01-04
Resolution : 3.90 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:

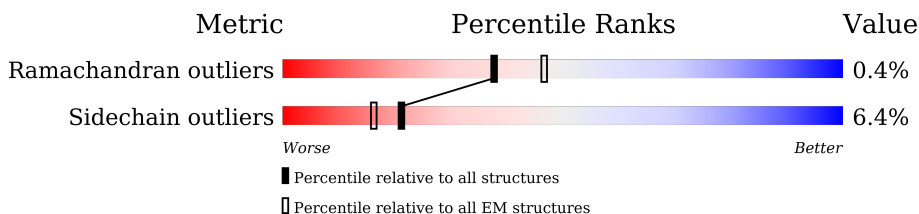
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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.






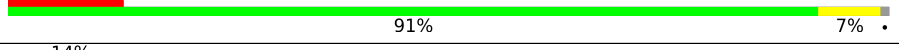
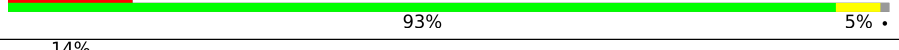
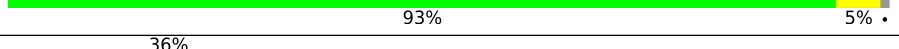
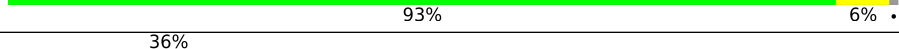
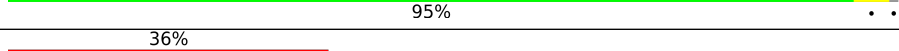
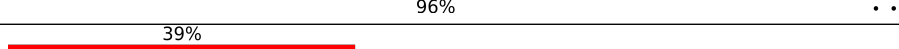
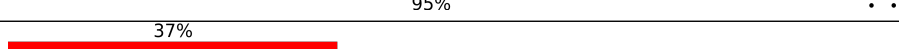
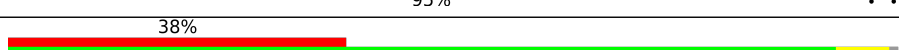
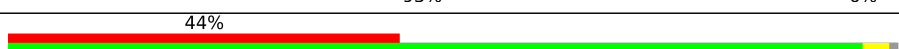
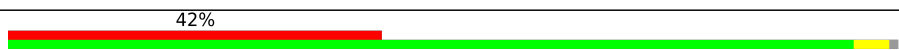
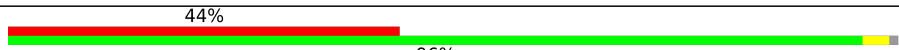
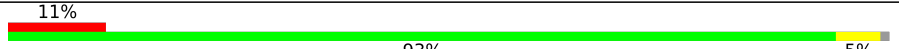
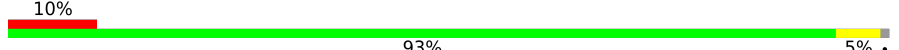
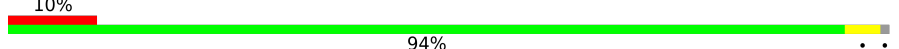
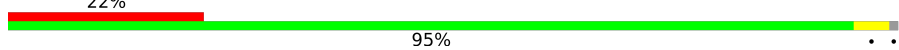
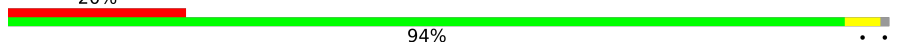
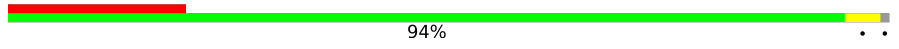
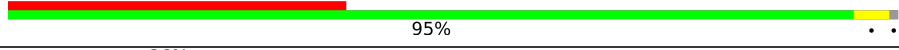
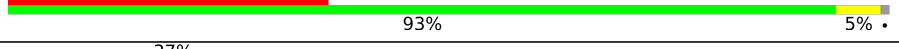
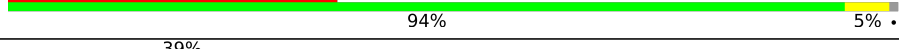


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	533	83% 6% 11%
1	B1	533	85% 0% 11%
1	B2	533	86% 0% 11%
1	B3	533	85% 0% 11%
1	B4	533	84% 5% 11%
1	B5	533	85% 0% 11%
1	b	533	85% 0% 11%
1	b1	533	84% 5% 11%
1	b2	533	85% 0% 11%

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Mol	Chain	Length	Quality of chain
1	b3	533	 86% 11%
1	b4	533	 84% 5% 11%
1	b5	533	 84% 5% 11%
2	O	246	 13% 91% 7%
2	O1	246	 14% 93% 5%
2	O2	246	 14% 93% 5%
2	P	246	 36% 93% 6%
2	P1	246	 36% 95%
2	P2	246	 36% 96%
2	Q	246	 39% 95%
2	Q1	246	 37% 95%
2	Q2	246	 38% 93% 6%
2	R	246	 44% 96%
2	R1	246	 42% 95%
2	R2	246	 44% 96%
2	V	246	 11% 93% 5%
2	V1	246	 10% 93% 5%
2	V2	246	 10% 94%
2	o	246	 22% 95%
2	o1	246	 20% 94%
2	o2	246	 20% 94%
2	p	246	 38% 95%
2	p1	246	 36% 93% 5%
2	p2	246	 37% 94% 5%
2	q	246	 39% 94%

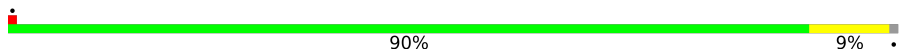
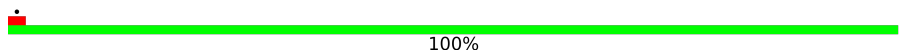
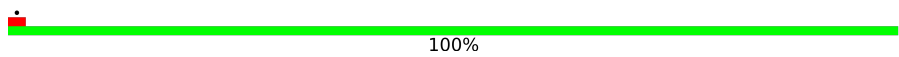

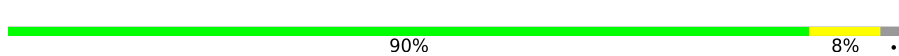
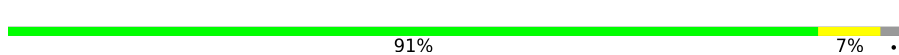


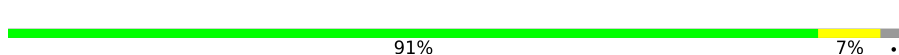
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Mol	Chain	Length	Quality of chain
2	q1	246	39% 95%
2	q2	246	40% 96%
2	r	246	43% 96%
2	r1	246	44% 95%
2	r2	246	42% 96%
2	v	246	13% 95%
2	v1	246	13% 95%
2	v2	246	13% 93% 6%
3	U	131	92% 7%
3	U1	131	90% 9%
3	U2	131	89% 10%
3	U3	131	88% 11%
3	U4	131	85% 13%
3	U5	131	89% 10%
4	W	68	91% 7%
4	W1	68	91% 7%
4	W2	68	84% 15%
4	W3	68	85% 13%
4	W4	68	93% 6%
4	W5	68	82% 16%
4	w	68	84% 15%
4	w1	68	90% 9%
4	w2	68	90% 9%
4	w3	68	87% 12%
4	w4	68	91% 7%

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Mol	Chain	Length	Quality of chain
4	w5	68	 90% 9%
5	DA	104	 100%
6	DB	92	 100%
7	f	117	 87% 10%
7	f1	117	 90% 8%
7	f2	117	 91% 7%
7	f3	117	 87% 10%
7	f4	117	 85% 12%
7	f5	117	 91% 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 120109 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 Portal protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	475	3727	2328	671	704	24	0	0
1	b	473	3710	2316	669	701	24	0	0
1	B1	475	3727	2328	671	704	24	0	0
1	b1	473	3710	2316	669	701	24	0	0
1	B2	475	3727	2328	671	704	24	0	0
1	b2	473	3710	2316	669	701	24	0	0
1	B3	475	3727	2328	671	704	24	0	0
1	b3	473	3710	2316	669	701	24	0	0
1	B4	475	3727	2328	671	704	24	0	0
1	b4	473	3710	2316	669	701	24	0	0
1	B5	475	3727	2328	671	704	24	0	0
1	b5	473	3710	2316	669	701	24	0	0

- Molecule 2 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	O	243	1792	1119	302	366	5	0	0
2	P	243	1792	1119	302	366	5	0	0
2	Q	243	1792	1119	302	366	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	V	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	v	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	V1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	v1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	V2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	v2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	o	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	O1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	o1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	O2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	o2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	p	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	P1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	p1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	P2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	p2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	q	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	Q1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	q1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	Q2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	q2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	r	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	R1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	r1	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	R2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0
2	r2	243	Total 1792	C 1119	N 302	O 366	S 5	0	0

- Molecule 3 is a protein called Tail tube terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	U	131	Total 1032	C 655	N 159	O 213	S 5	0	0
3	U1	131	Total 1032	C 655	N 159	O 213	S 5	0	0
3	U2	131	Total 1032	C 655	N 159	O 213	S 5	0	0
3	U3	131	Total 1032	C 655	N 159	O 213	S 5	0	0
3	U4	131	Total 1032	C 655	N 159	O 213	S 5	0	0
3	U5	131	Total 1032	C 655	N 159	O 213	S 5	0	0

- Molecule 4 is a protein called Head completion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	W	67	Total 524	C 323	N 101	O 98	S 2	0	0
4	w	67	Total 524	C 323	N 101	O 98	S 2	0	0
4	W1	67	Total 524	C 323	N 101	O 98	S 2	0	0
4	w1	67	Total 524	C 323	N 101	O 98	S 2	0	0
4	W2	67	Total 524	C 323	N 101	O 98	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	w2	67	Total	C	N	O	S	0	0
			524	323	101	98	2		
4	W3	67	Total	C	N	O	S	0	0
			524	323	101	98	2		
4	w3	67	Total	C	N	O	S	0	0
			524	323	101	98	2		
4	W4	67	Total	C	N	O	S	0	0
			524	323	101	98	2		
4	w4	67	Total	C	N	O	S	0	0
			524	323	101	98	2		
4	W5	67	Total	C	N	O	S	0	0
			524	323	101	98	2		
4	w5	67	Total	C	N	O	S	0	0
			524	323	101	98	2		

- Molecule 5 is a DNA chain called DNA (104-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DA	104	Total	C	N	O	P	0	0
			2128	1010	400	614	104		

- Molecule 6 is a DNA chain called DNA (92-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DB	92	Total	C	N	O	P	0	0
			1887	900	333	562	92		

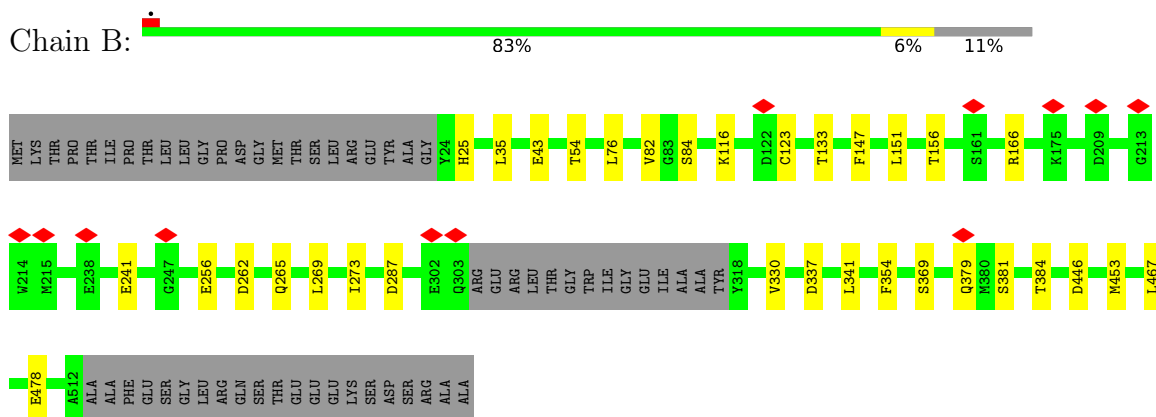
- Molecule 7 is a protein called Head-tail connector protein FII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	114	Total	C	N	O	S	0	0
			872	535	161	174	2		
7	f1	114	Total	C	N	O	S	0	0
			872	535	161	174	2		
7	f2	114	Total	C	N	O	S	0	0
			872	535	161	174	2		
7	f3	114	Total	C	N	O	S	0	0
			872	535	161	174	2		
7	f4	114	Total	C	N	O	S	0	0
			872	535	161	174	2		
7	f5	114	Total	C	N	O	S	0	0
			872	535	161	174	2		

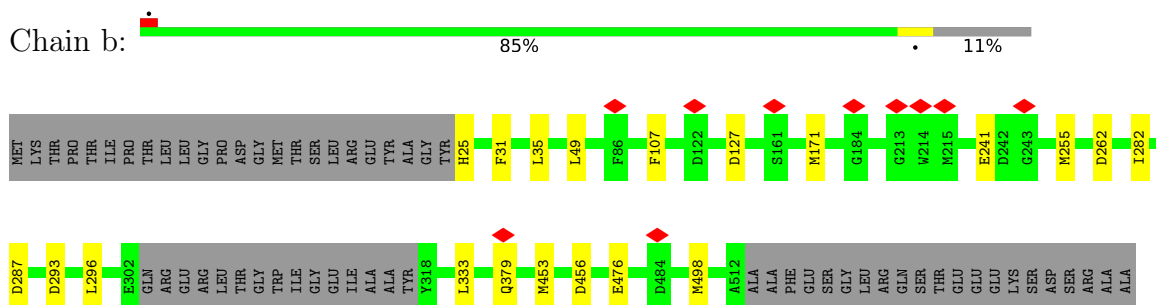
3 Residue-property plots [i](#)

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.

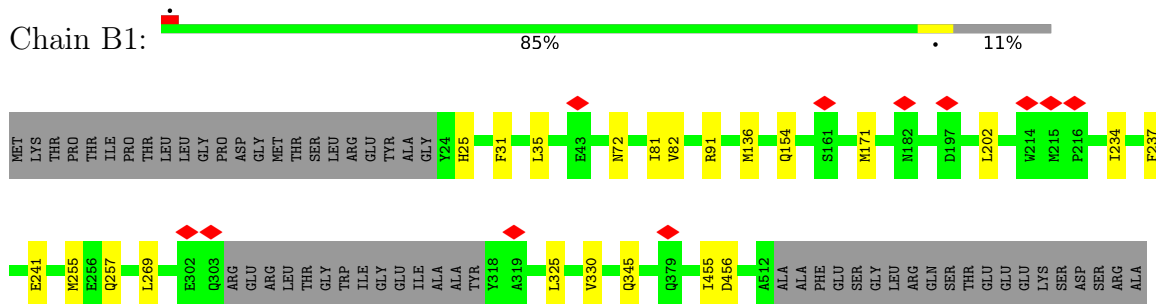
- Molecule 1: Portal protein B



- Molecule 1: Portal protein B



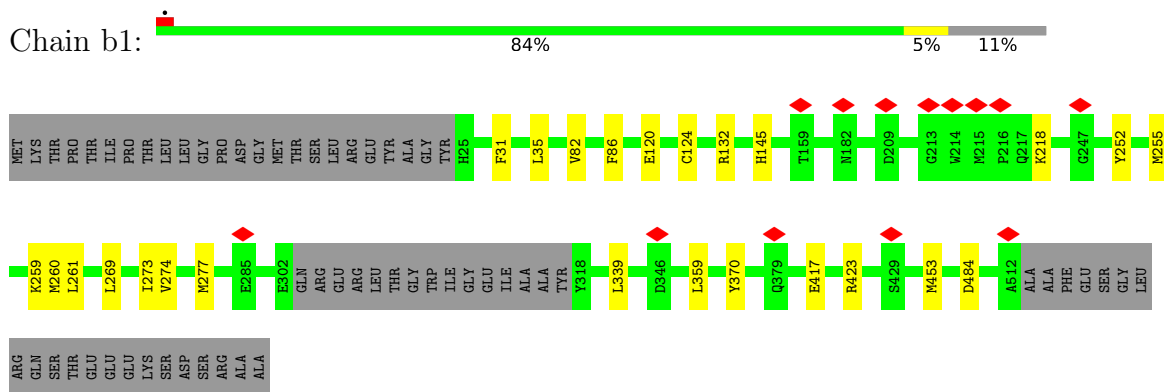
- Molecule 1: Portal protein B



ALA

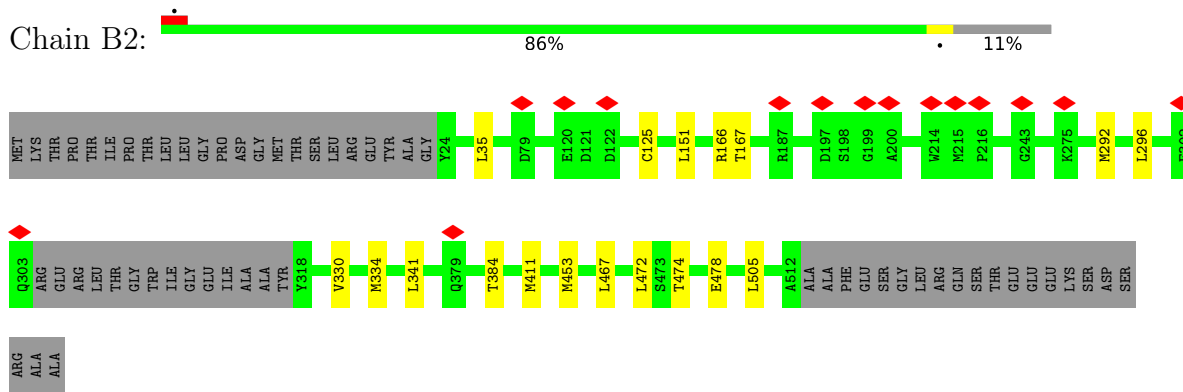
• Molecule 1: Portal protein B

Chain b1:



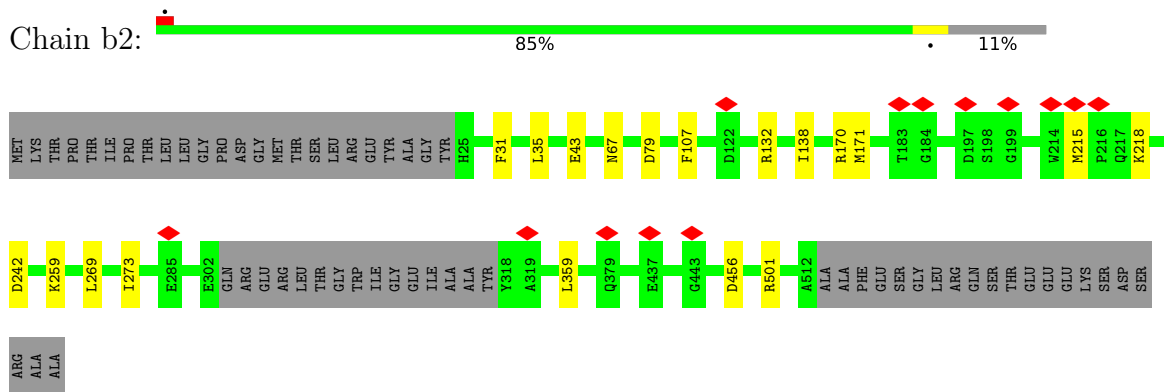
• Molecule 1: Portal protein B

Chain B2:



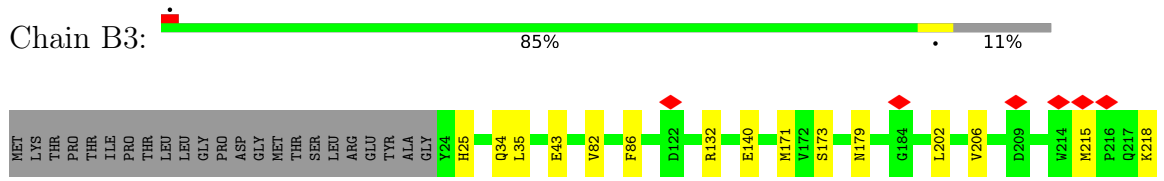
• Molecule 1: Portal protein B

Chain b2:



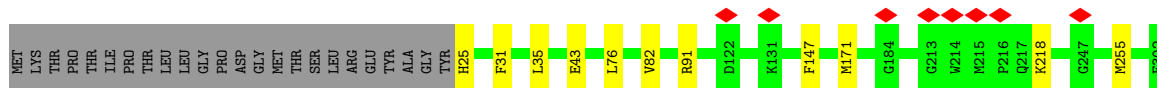
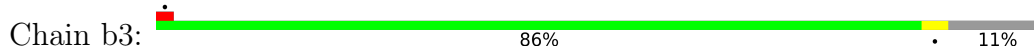
• Molecule 1: Portal protein B

Chain B3:

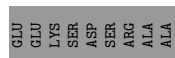
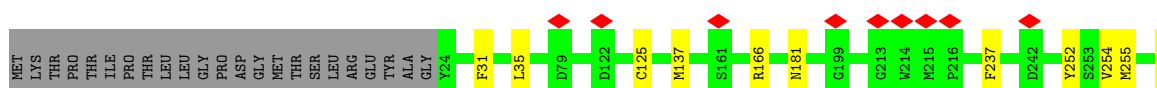
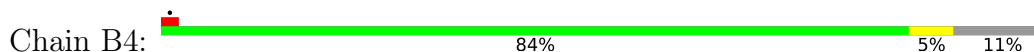




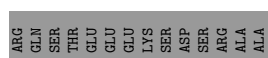
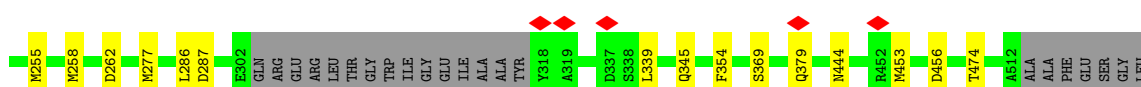
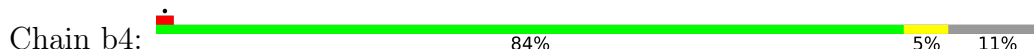
• Molecule 1: Portal protein B



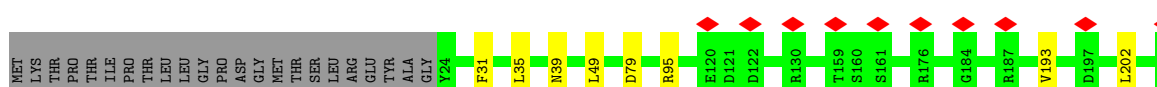
• Molecule 1: Portal protein B

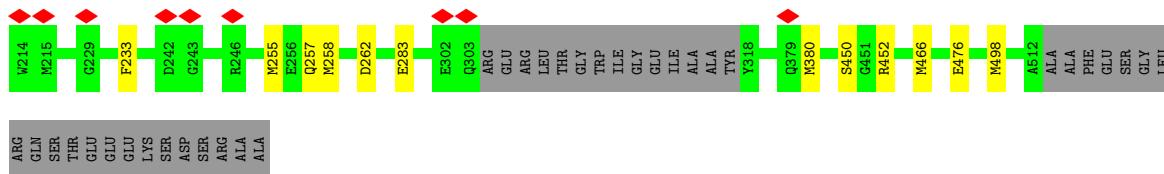


• Molecule 1: Portal protein B

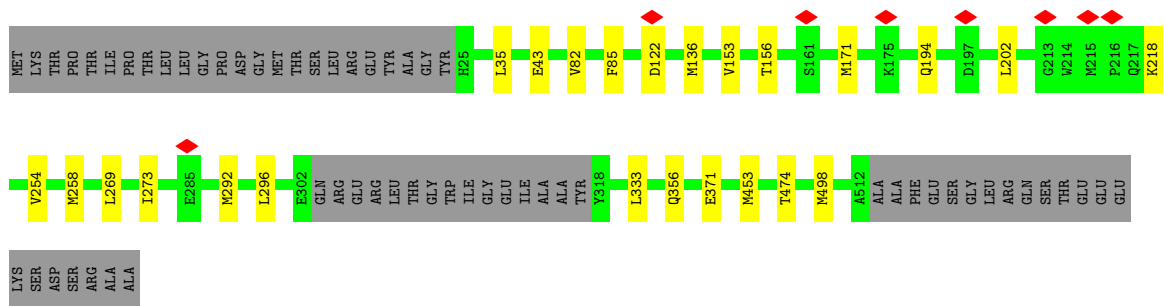
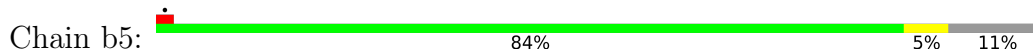


• Molecule 1: Portal protein B

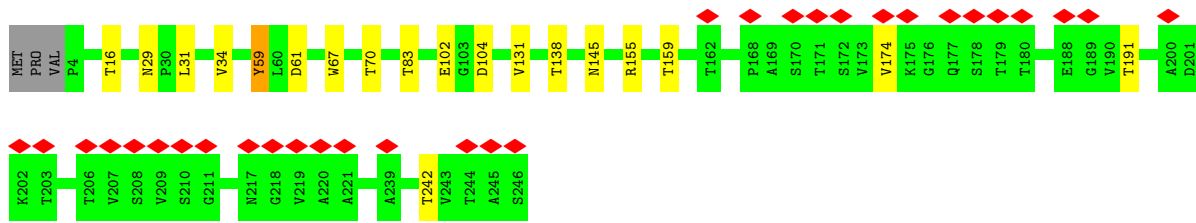
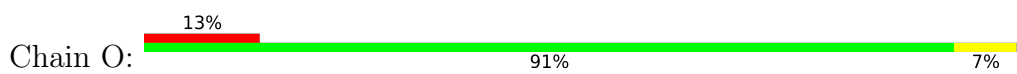




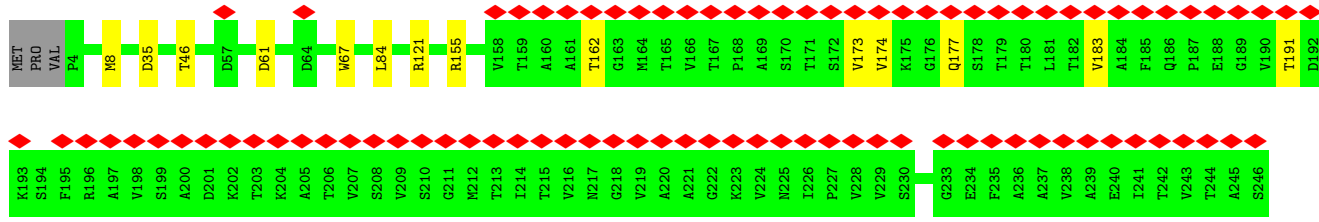
• Molecule 1: Portal protein B



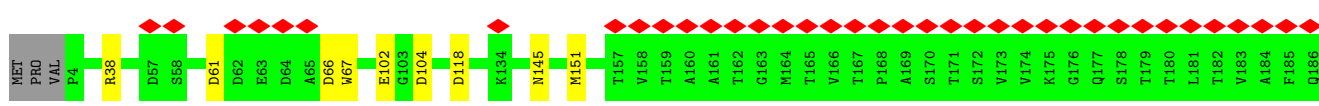
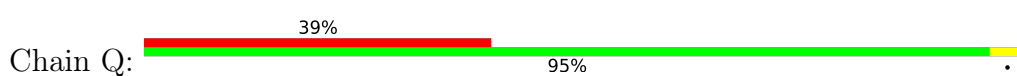
• Molecule 2: Tail tube protein

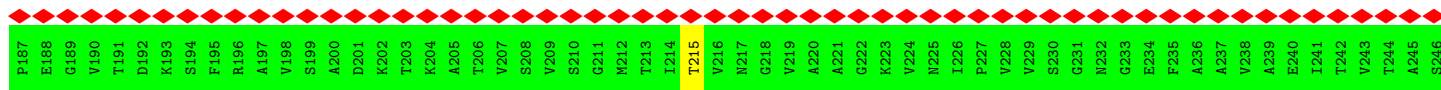


• Molecule 2: Tail tube protein

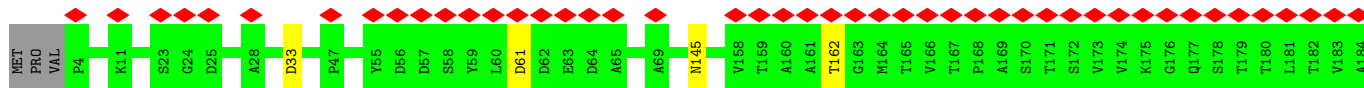
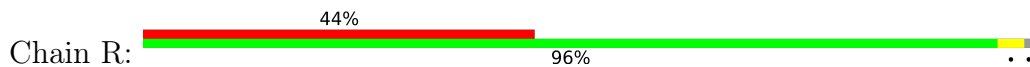


• Molecule 2: Tail tube protein

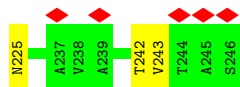
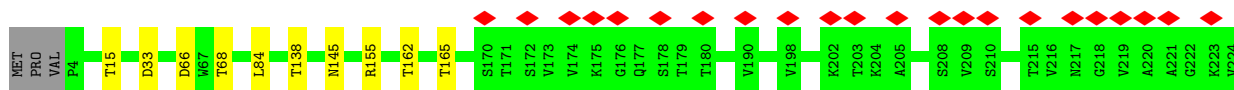




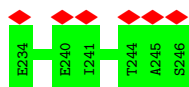
• Molecule 2: Tail tube protein



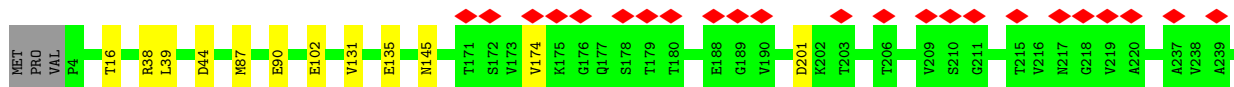
• Molecule 2: Tail tube protein



• Molecule 2: Tail tube protein

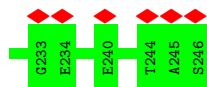


• Molecule 2: Tail tube protein

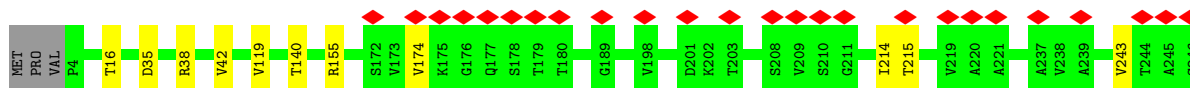




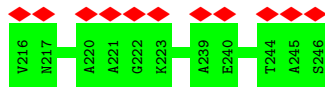
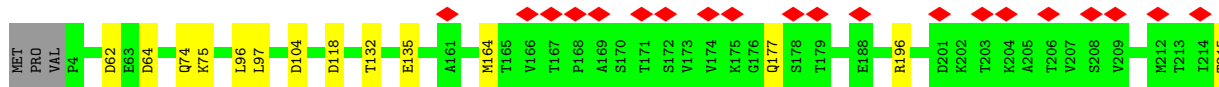
• Molecule 2: Tail tube protein



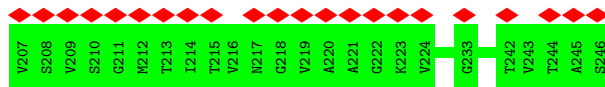
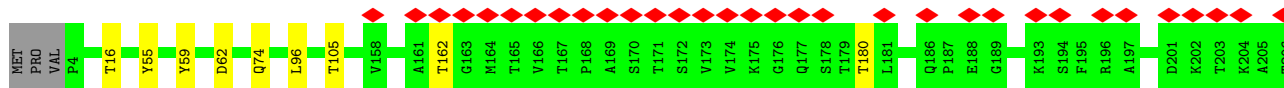
• Molecule 2: Tail tube protein



• Molecule 2: Tail tube protein

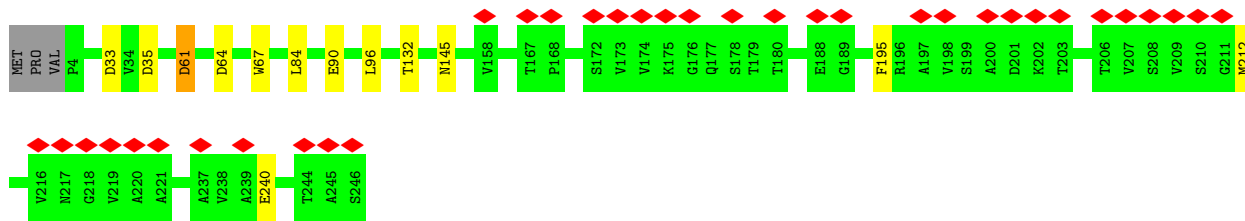


• Molecule 2: Tail tube protein

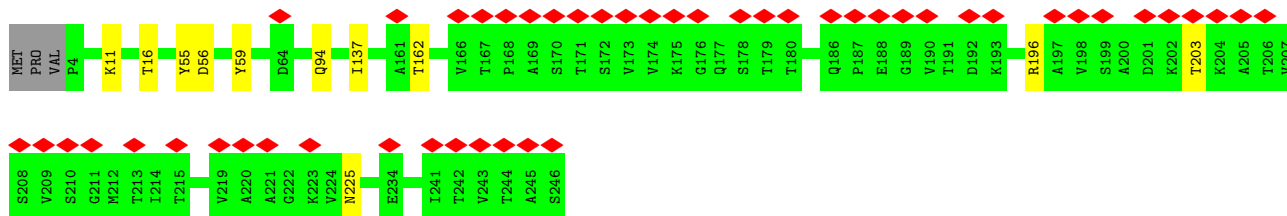


• Molecule 2: Tail tube protein

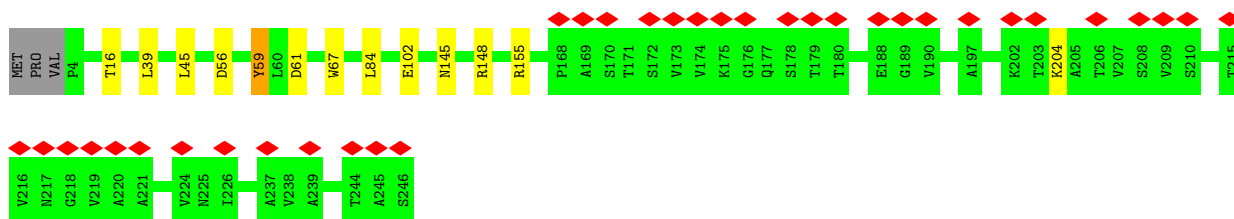




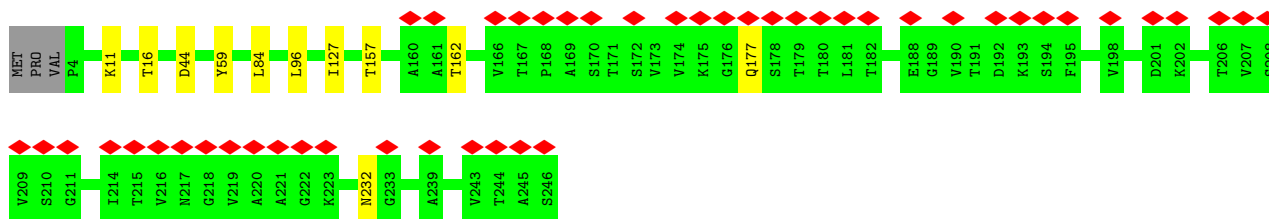
• Molecule 2: Tail tube protein



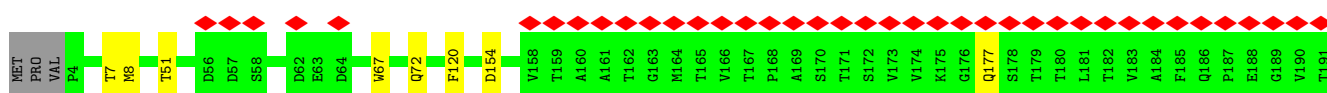
• Molecule 2: Tail tube protein

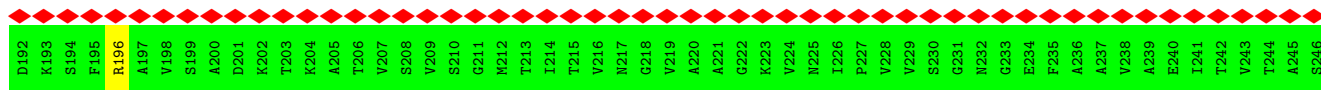


• Molecule 2: Tail tube protein

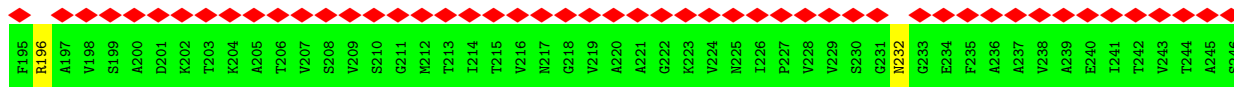
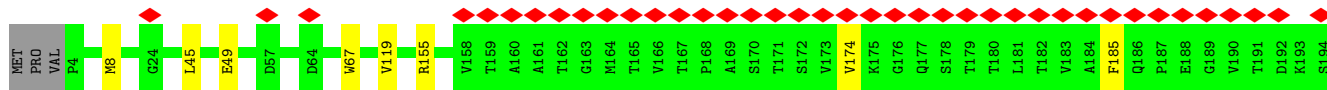


• Molecule 2: Tail tube protein

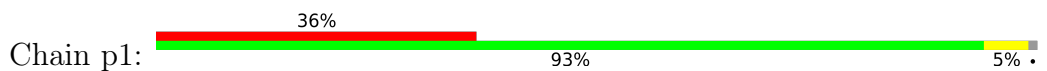




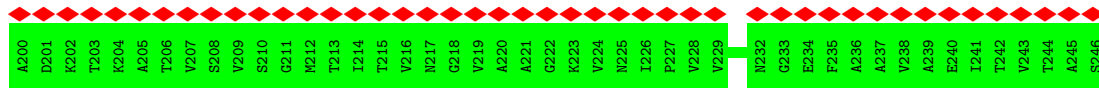
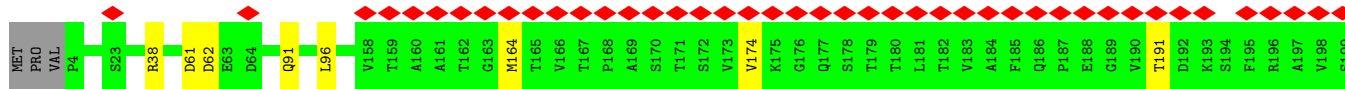
• Molecule 2: Tail tube protein



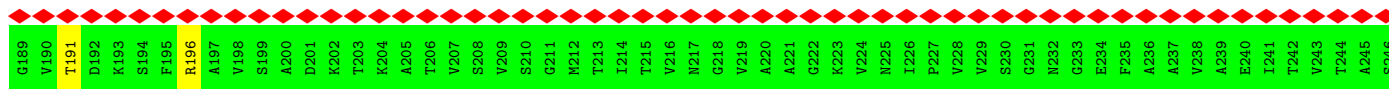
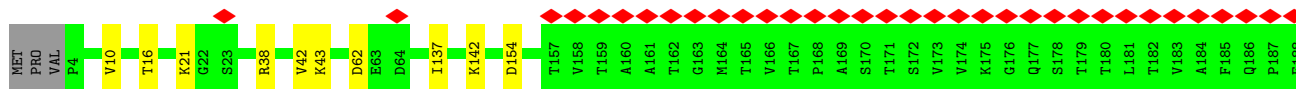
• Molecule 2: Tail tube protein



• Molecule 2: Tail tube protein

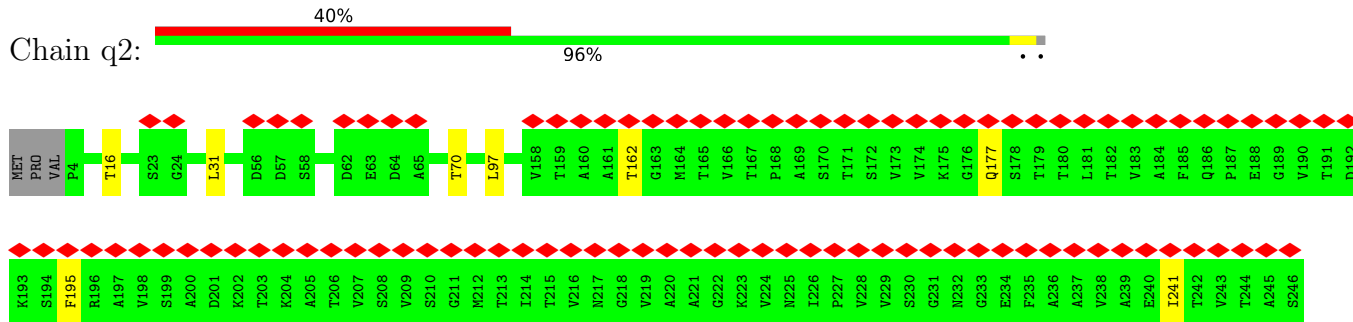


• Molecule 2: Tail tube protein

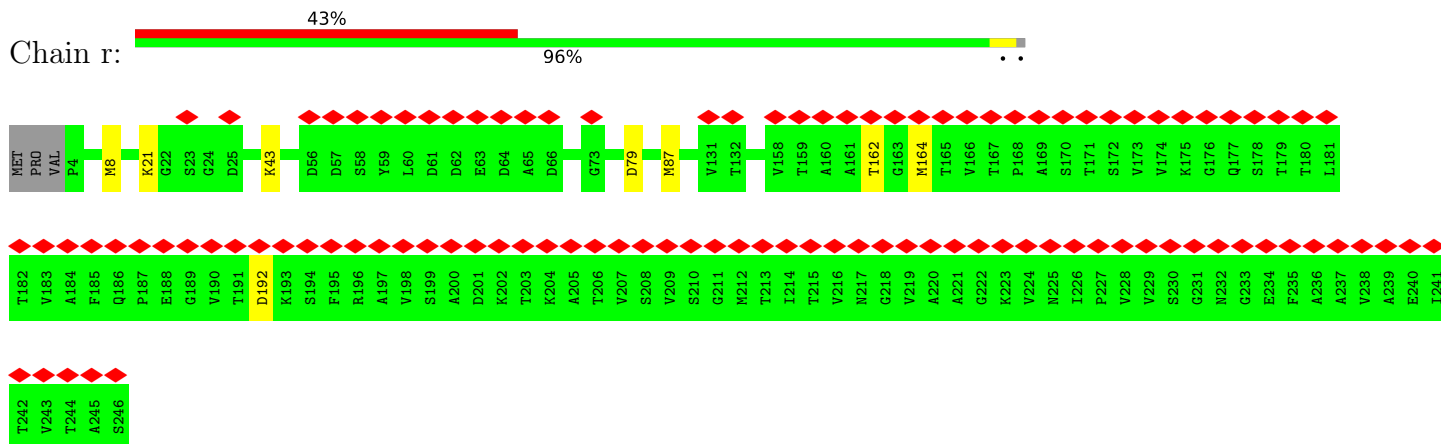


• Molecule 2: Tail tube protein

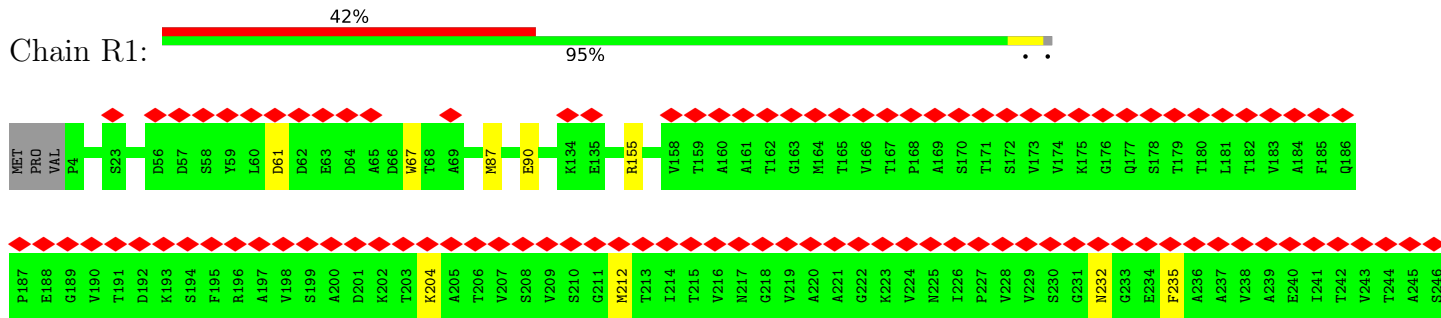
• Molecule 2: Tail tube protein



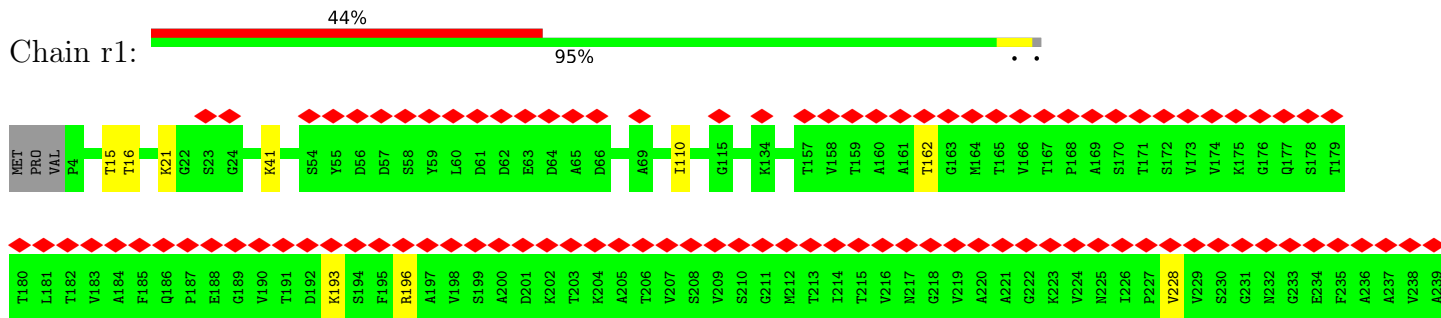
• Molecule 2: Tail tube protein

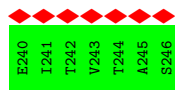


• Molecule 2: Tail tube protein

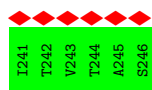
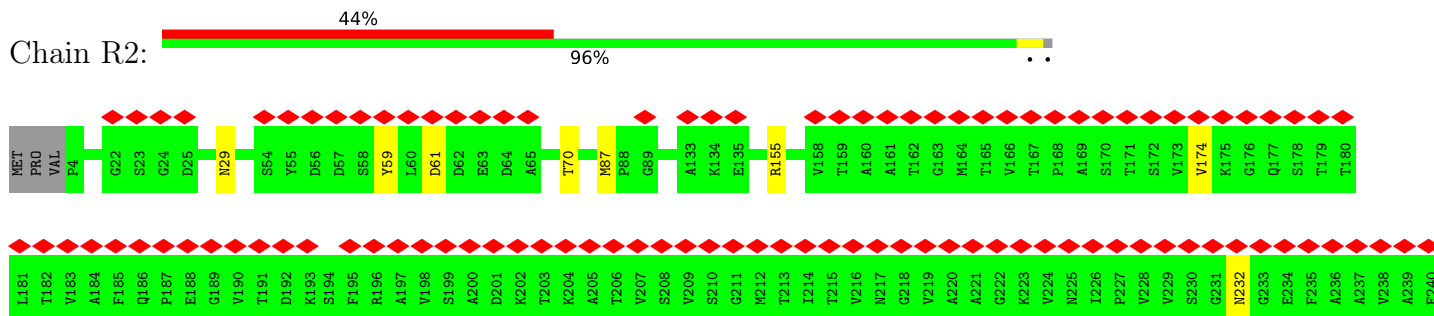


• Molecule 2: Tail tube protein

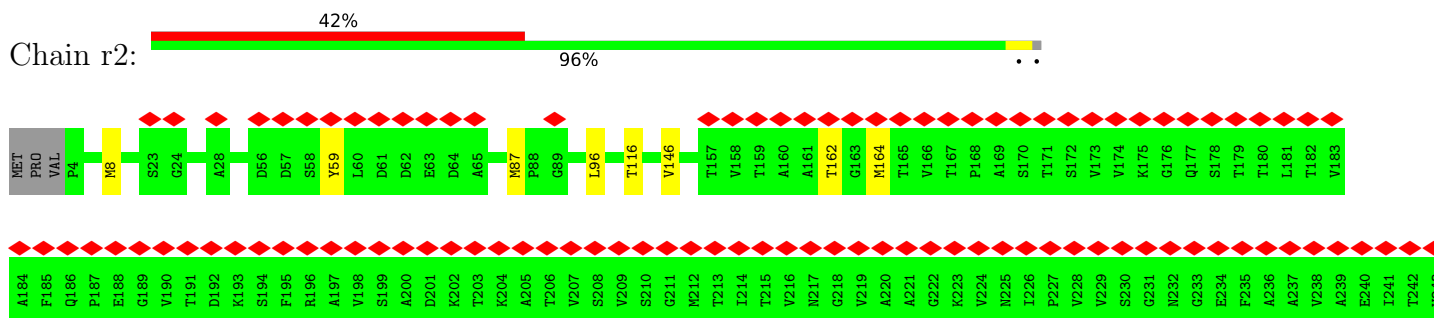




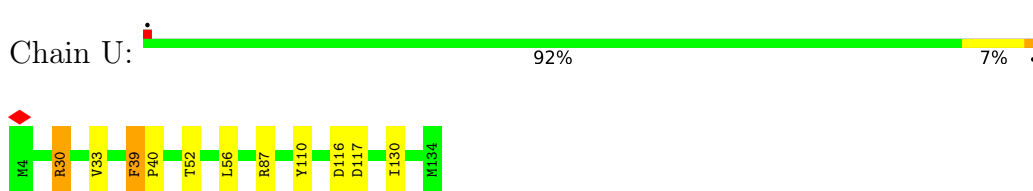
• Molecule 2: Tail tube protein



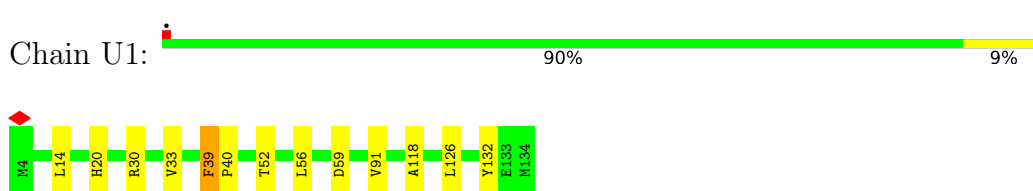
• Molecule 2: Tail tube protein



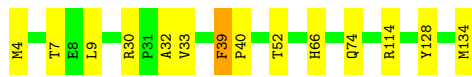
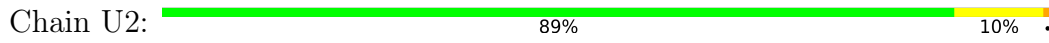
• Molecule 3: Tail tube terminator protein



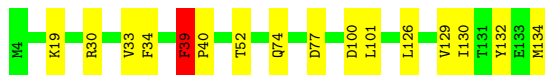
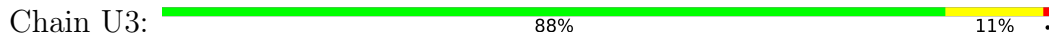
• Molecule 3: Tail tube terminator protein



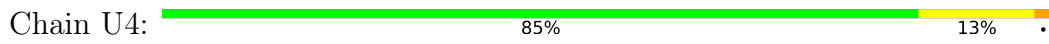
• Molecule 3: Tail tube terminator protein



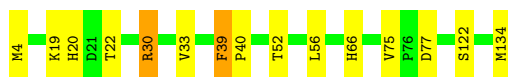
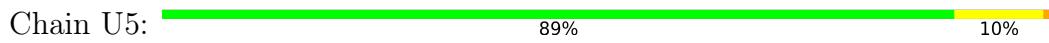
• Molecule 3: Tail tube terminator protein



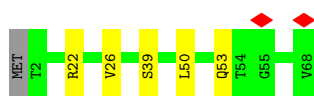
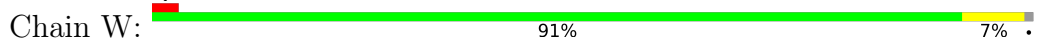
• Molecule 3: Tail tube terminator protein



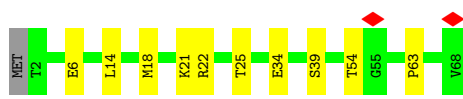
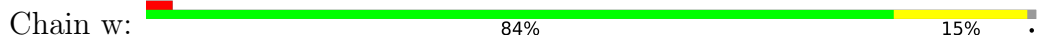
• Molecule 3: Tail tube terminator protein



• Molecule 4: Head completion protein



• Molecule 4: Head completion protein



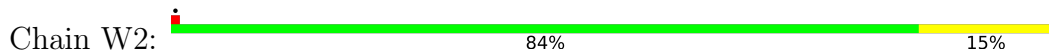
• Molecule 4: Head completion protein



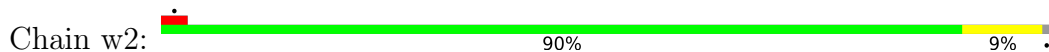
• Molecule 4: Head completion protein



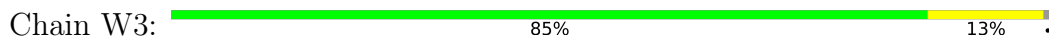
● Molecule 4: Head completion protein



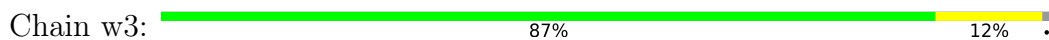
● Molecule 4: Head completion protein



● Molecule 4: Head completion protein



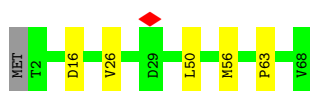
● Molecule 4: Head completion protein




● Molecule 4: Head completion protein



● Molecule 4: Head completion protein



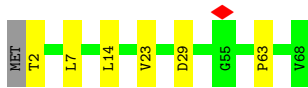
● Molecule 4: Head completion protein

Chain W5:  82% 16%



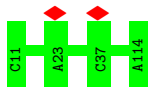
- Molecule 4: Head completion protein

Chain w5:  90% 9%



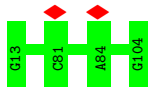
- Molecule 5: DNA (104-MER)

Chain DA:  100%




- Molecule 6: DNA (92-MER)

Chain DB:  100%




- Molecule 7: Head-tail connector protein FII

Chain f:  87% 10%




- Molecule 7: Head-tail connector protein FII

Chain f1:  90% 8%




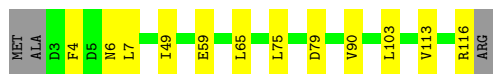
- Molecule 7: Head-tail connector protein FII

Chain f2:  91% 7%




- Molecule 7: Head-tail connector protein FII

Chain f3:  87% 10%




- Molecule 7: Head-tail connector protein FII

Chain f4:  85% 12%



- Molecule 7: Head-tail connector protein FII

Chain f5:  91% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.199	Depositor
Minimum map value	-1.385	Depositor
Average map value	-0.016	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.52	Depositor
Map size (\AA)	515.616, 515.616, 515.616	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.29	0/3811	0.51	0/5151
1	B1	0.28	0/3811	0.50	0/5151
1	B2	0.28	0/3811	0.51	0/5151
1	B3	0.28	0/3811	0.51	0/5151
1	B4	0.28	0/3811	0.50	0/5151
1	B5	0.29	0/3811	0.50	0/5151
1	b	0.29	0/3793	0.51	0/5126
1	b1	0.28	0/3793	0.50	0/5126
1	b2	0.28	0/3793	0.50	0/5126
1	b3	0.28	0/3793	0.50	0/5126
1	b4	0.28	0/3793	0.50	0/5126
1	b5	0.28	0/3793	0.50	0/5126
2	O	2.74	6/1827 (0.3%)	0.55	1/2494 (0.0%)
2	O1	0.27	0/1827	0.51	0/2494
2	O2	2.76	6/1827 (0.3%)	0.55	1/2494 (0.0%)
2	P	0.27	0/1827	0.52	0/2494
2	P1	0.26	0/1827	0.50	0/2494
2	P2	0.27	0/1827	0.52	0/2494
2	Q	0.26	0/1827	0.52	0/2494
2	Q1	0.26	0/1827	0.49	0/2494
2	Q2	0.25	0/1827	0.51	0/2494
2	R	0.25	0/1827	0.50	0/2494
2	R1	0.25	0/1827	0.51	0/2494
2	R2	0.25	0/1827	0.51	0/2494
2	V	0.28	0/1827	0.53	0/2494
2	V1	0.29	0/1827	0.51	0/2494
2	V2	0.28	0/1827	0.52	0/2494
2	o	0.28	0/1827	0.53	0/2494
2	o1	0.27	0/1827	0.52	0/2494
2	o2	0.27	0/1827	0.52	0/2494
2	p	0.26	0/1827	0.51	0/2494
2	p1	0.41	2/1827 (0.1%)	0.59	1/2494 (0.0%)
2	p2	0.41	2/1827 (0.1%)	0.59	1/2494 (0.0%)
2	q	0.26	0/1827	0.51	0/2494

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	q1	0.26	0/1827	0.51	0/2494
2	q2	0.25	0/1827	0.50	0/2494
2	r	0.25	0/1827	0.50	0/2494
2	r1	0.25	0/1827	0.52	0/2494
2	r2	0.25	0/1827	0.51	0/2494
2	v	0.28	0/1827	0.51	0/2494
2	v1	0.28	0/1827	0.51	0/2494
2	v2	0.28	0/1827	0.51	0/2494
3	U	0.31	0/1058	0.52	0/1444
3	U1	0.31	0/1058	0.50	0/1444
3	U2	0.30	0/1058	0.51	0/1444
3	U3	0.31	0/1058	0.50	0/1444
3	U4	0.30	0/1058	0.51	0/1444
3	U5	0.31	0/1058	0.51	0/1444
4	W	0.29	0/529	0.57	0/709
4	W1	0.28	0/529	0.57	0/709
4	W2	0.28	0/529	0.57	0/709
4	W3	0.29	0/529	0.59	0/709
4	W4	0.29	0/529	0.55	0/709
4	W5	0.30	0/529	0.59	0/709
4	w	0.30	0/529	0.60	0/709
4	w1	0.30	0/529	0.59	0/709
4	w2	0.29	0/529	0.59	0/709
4	w3	0.30	0/529	0.58	0/709
4	w4	0.30	0/529	0.57	0/709
4	w5	0.29	0/529	0.59	0/709
5	DA	0.52	0/2389	0.90	0/3682
6	DB	0.52	0/2113	0.95	0/3261
7	f	0.30	0/888	0.59	0/1204
7	f1	0.30	0/888	0.58	0/1204
7	f2	0.28	0/888	0.58	0/1204
7	f3	0.29	0/888	0.57	0/1204
7	f4	0.28	0/888	0.57	0/1204
7	f5	0.28	0/888	0.56	0/1204
All	All	0.56	16/122960 (0.0%)	0.54	4/167821 (0.0%)

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
3	U	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	U1	0	1
3	U2	0	1
3	U3	0	1
3	U4	0	1
3	U5	0	1
All	All	0	6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O2	59	TYR	CD1-CE1	66.16	2.38	1.39
2	O	59	TYR	CD1-CE1	64.66	2.36	1.39
2	O2	59	TYR	CD2-CE2	62.46	2.33	1.39
2	O	59	TYR	CD2-CE2	61.93	2.32	1.39
2	O	59	TYR	CE1-CZ	41.96	1.93	1.38
2	O	59	TYR	CE2-CZ	41.72	1.92	1.38
2	O2	59	TYR	CE2-CZ	41.45	1.92	1.38
2	O2	59	TYR	CE1-CZ	41.23	1.92	1.38
2	O	59	TYR	CG-CD1	32.86	1.81	1.39
2	O2	59	TYR	CG-CD1	32.45	1.81	1.39
2	O	59	TYR	CG-CD2	31.95	1.80	1.39
2	O2	59	TYR	CG-CD2	31.85	1.80	1.39
2	p2	42	VAL	C-N	10.84	1.58	1.34
2	p1	42	VAL	C-N	10.83	1.58	1.34
2	p1	43	LYS	N-CA	7.89	1.62	1.46
2	p2	43	LYS	N-CA	7.81	1.61	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	p2	42	VAL	C-N-CA	12.32	152.49	121.70
2	p1	42	VAL	C-N-CA	12.25	152.32	121.70
2	O	59	TYR	CB-CG-CD2	-5.27	117.84	121.00
2	O2	59	TYR	CB-CG-CD2	-5.01	118.00	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	U	39	PHE	Peptide
3	U1	39	PHE	Peptide

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Mol	Chain	Res	Type	Group
3	U2	39	PHE	Peptide
3	U3	39	PHE	Peptide
3	U4	39	PHE	Peptide
3	U5	39	PHE	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	B	471/533 (88%)	445 (94%)	26 (6%)	0	100	100
1	B1	471/533 (88%)	436 (93%)	35 (7%)	0	100	100
1	B2	471/533 (88%)	438 (93%)	33 (7%)	0	100	100
1	B3	471/533 (88%)	433 (92%)	37 (8%)	1 (0%)	47	79
1	B4	471/533 (88%)	434 (92%)	36 (8%)	1 (0%)	47	79
1	B5	471/533 (88%)	436 (93%)	35 (7%)	0	100	100
1	b	469/533 (88%)	446 (95%)	23 (5%)	0	100	100
1	b1	469/533 (88%)	437 (93%)	32 (7%)	0	100	100
1	b2	469/533 (88%)	441 (94%)	28 (6%)	0	100	100
1	b3	469/533 (88%)	433 (92%)	36 (8%)	0	100	100
1	b4	469/533 (88%)	443 (94%)	25 (5%)	1 (0%)	47	79
1	b5	469/533 (88%)	441 (94%)	28 (6%)	0	100	100
2	O	241/246 (98%)	220 (91%)	19 (8%)	2 (1%)	19	57
2	O1	241/246 (98%)	214 (89%)	26 (11%)	1 (0%)	34	71
2	O2	241/246 (98%)	221 (92%)	19 (8%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	241/246 (98%)	218 (90%)	21 (9%)	2 (1%)	19	57
2	P1	241/246 (98%)	219 (91%)	22 (9%)	0	100	100
2	P2	241/246 (98%)	215 (89%)	25 (10%)	1 (0%)	34	71
2	Q	241/246 (98%)	216 (90%)	24 (10%)	1 (0%)	34	71
2	Q1	241/246 (98%)	219 (91%)	21 (9%)	1 (0%)	34	71
2	Q2	241/246 (98%)	222 (92%)	18 (8%)	1 (0%)	34	71
2	R	241/246 (98%)	216 (90%)	24 (10%)	1 (0%)	34	71
2	R1	241/246 (98%)	220 (91%)	20 (8%)	1 (0%)	34	71
2	R2	241/246 (98%)	217 (90%)	23 (10%)	1 (0%)	34	71
2	V	241/246 (98%)	222 (92%)	19 (8%)	0	100	100
2	V1	241/246 (98%)	218 (90%)	23 (10%)	0	100	100
2	V2	241/246 (98%)	211 (88%)	30 (12%)	0	100	100
2	o	241/246 (98%)	219 (91%)	22 (9%)	0	100	100
2	o1	241/246 (98%)	220 (91%)	21 (9%)	0	100	100
2	o2	241/246 (98%)	219 (91%)	21 (9%)	1 (0%)	34	71
2	p	241/246 (98%)	217 (90%)	23 (10%)	1 (0%)	34	71
2	p1	241/246 (98%)	217 (90%)	23 (10%)	1 (0%)	34	71
2	p2	241/246 (98%)	219 (91%)	22 (9%)	0	100	100
2	q	241/246 (98%)	221 (92%)	20 (8%)	0	100	100
2	q1	241/246 (98%)	219 (91%)	21 (9%)	1 (0%)	34	71
2	q2	241/246 (98%)	222 (92%)	18 (8%)	1 (0%)	34	71
2	r	241/246 (98%)	220 (91%)	21 (9%)	0	100	100
2	r1	241/246 (98%)	219 (91%)	22 (9%)	0	100	100
2	r2	241/246 (98%)	221 (92%)	19 (8%)	1 (0%)	34	71
2	v	241/246 (98%)	225 (93%)	15 (6%)	1 (0%)	34	71
2	v1	241/246 (98%)	220 (91%)	20 (8%)	1 (0%)	34	71
2	v2	241/246 (98%)	221 (92%)	19 (8%)	1 (0%)	34	71
3	U	129/131 (98%)	107 (83%)	19 (15%)	3 (2%)	6	38
3	U1	129/131 (98%)	102 (79%)	23 (18%)	4 (3%)	4	32
3	U2	129/131 (98%)	104 (81%)	21 (16%)	4 (3%)	4	32
3	U3	129/131 (98%)	105 (81%)	20 (16%)	4 (3%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	U4	129/131 (98%)	102 (79%)	24 (19%)	3 (2%)	6	38
3	U5	129/131 (98%)	111 (86%)	15 (12%)	3 (2%)	6	38
4	W	65/68 (96%)	61 (94%)	4 (6%)	0	100	100
4	W1	65/68 (96%)	61 (94%)	4 (6%)	0	100	100
4	W2	65/68 (96%)	60 (92%)	4 (6%)	1 (2%)	10	45
4	W3	65/68 (96%)	58 (89%)	6 (9%)	1 (2%)	10	45
4	W4	65/68 (96%)	59 (91%)	6 (9%)	0	100	100
4	W5	65/68 (96%)	58 (89%)	6 (9%)	1 (2%)	10	45
4	w	65/68 (96%)	60 (92%)	4 (6%)	1 (2%)	10	45
4	w1	65/68 (96%)	60 (92%)	4 (6%)	1 (2%)	10	45
4	w2	65/68 (96%)	57 (88%)	7 (11%)	1 (2%)	10	45
4	w3	65/68 (96%)	59 (91%)	5 (8%)	1 (2%)	10	45
4	w4	65/68 (96%)	57 (88%)	7 (11%)	1 (2%)	10	45
4	w5	65/68 (96%)	58 (89%)	6 (9%)	1 (2%)	10	45
7	f	112/117 (96%)	97 (87%)	15 (13%)	0	100	100
7	f1	112/117 (96%)	95 (85%)	17 (15%)	0	100	100
7	f2	112/117 (96%)	90 (80%)	21 (19%)	1 (1%)	17	54
7	f3	112/117 (96%)	94 (84%)	18 (16%)	0	100	100
7	f4	112/117 (96%)	92 (82%)	20 (18%)	0	100	100
7	f5	112/117 (96%)	91 (81%)	21 (19%)	0	100	100
All	All	15096/16080 (94%)	13728 (91%)	1312 (9%)	56 (0%)	38	71

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	61	ASP
2	P	61	ASP
2	Q	61	ASP
3	U	30	ARG
4	w	63	PRO
4	w1	63	PRO
4	W2	63	PRO
4	w2	63	PRO
3	U2	30	ARG
3	U2	33	VAL

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Mol	Chain	Res	Type
4	W3	63	PRO
4	w3	63	PRO
3	U3	30	ARG
4	w4	63	PRO
4	W5	63	PRO
4	w5	63	PRO
2	O2	61	ASP
2	P2	61	ASP
2	Q1	61	ASP
2	R2	61	ASP
3	U5	30	ARG
2	O1	61	ASP
2	p1	59	TYR
2	Q2	61	ASP
2	R1	61	ASP
3	U1	30	ARG
3	U1	118	ALA
3	U4	30	ARG
2	v	177	GLN
2	v1	177	GLN
2	o2	177	GLN
2	q1	177	GLN
2	R	61	ASP
3	U	40	PRO
3	U3	40	PRO
2	q2	177	GLN
3	U	33	VAL
3	U1	33	VAL
3	U1	40	PRO
7	f2	25	THR
3	U2	40	PRO
3	U3	33	VAL
1	B3	328	ALA
3	U4	33	VAL
3	U4	40	PRO
1	B4	328	ALA
1	b4	34	GLN
3	U5	33	VAL
2	v2	177	GLN
2	P	177	GLN
3	U2	32	ALA
2	p	177	GLN

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Mol	Chain	Res	Type
2	r2	59	TYR
2	O	34	VAL
3	U5	40	PRO
3	U3	39	PHE

5.3.2 Protein sidechains [i](#)

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	B	381/428 (89%)	348 (91%)	33 (9%)	10	37
1	B1	381/428 (89%)	359 (94%)	22 (6%)	20	50
1	B2	381/428 (89%)	363 (95%)	18 (5%)	26	55
1	B3	381/428 (89%)	359 (94%)	22 (6%)	20	50
1	B4	381/428 (89%)	357 (94%)	24 (6%)	18	47
1	B5	381/428 (89%)	361 (95%)	20 (5%)	23	53
1	b	380/428 (89%)	360 (95%)	20 (5%)	22	52
1	b1	380/428 (89%)	355 (93%)	25 (7%)	16	46
1	b2	380/428 (89%)	361 (95%)	19 (5%)	24	53
1	b3	380/428 (89%)	363 (96%)	17 (4%)	27	56
1	b4	380/428 (89%)	354 (93%)	26 (7%)	16	45
1	b5	380/428 (89%)	356 (94%)	24 (6%)	18	47
2	O	193/196 (98%)	176 (91%)	17 (9%)	10	37
2	O1	193/196 (98%)	180 (93%)	13 (7%)	16	46
2	O2	193/196 (98%)	181 (94%)	12 (6%)	18	48
2	P	193/196 (98%)	181 (94%)	12 (6%)	18	48
2	P1	193/196 (98%)	183 (95%)	10 (5%)	23	53
2	P2	193/196 (98%)	186 (96%)	7 (4%)	35	61
2	Q	193/196 (98%)	184 (95%)	9 (5%)	26	55
2	Q1	193/196 (98%)	185 (96%)	8 (4%)	30	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q2	193/196 (98%)	179 (93%)	14 (7%)	14	43
2	R	193/196 (98%)	187 (97%)	6 (3%)	40	64
2	R1	193/196 (98%)	185 (96%)	8 (4%)	30	58
2	R2	193/196 (98%)	186 (96%)	7 (4%)	35	61
2	V	193/196 (98%)	180 (93%)	13 (7%)	16	46
2	V1	193/196 (98%)	180 (93%)	13 (7%)	16	46
2	V2	193/196 (98%)	182 (94%)	11 (6%)	20	50
2	o	193/196 (98%)	184 (95%)	9 (5%)	26	55
2	o1	193/196 (98%)	182 (94%)	11 (6%)	20	50
2	o2	193/196 (98%)	183 (95%)	10 (5%)	23	53
2	p	193/196 (98%)	185 (96%)	8 (4%)	30	58
2	p1	193/196 (98%)	181 (94%)	12 (6%)	18	48
2	p2	193/196 (98%)	183 (95%)	10 (5%)	23	53
2	q	193/196 (98%)	182 (94%)	11 (6%)	20	50
2	q1	193/196 (98%)	185 (96%)	8 (4%)	30	58
2	q2	193/196 (98%)	186 (96%)	7 (4%)	35	61
2	r	193/196 (98%)	185 (96%)	8 (4%)	30	58
2	r1	193/196 (98%)	184 (95%)	9 (5%)	26	55
2	r2	193/196 (98%)	186 (96%)	7 (4%)	35	61
2	v	193/196 (98%)	184 (95%)	9 (5%)	26	55
2	v1	193/196 (98%)	184 (95%)	9 (5%)	26	55
2	v2	193/196 (98%)	180 (93%)	13 (7%)	16	46
3	U	109/109 (100%)	100 (92%)	9 (8%)	11	39
3	U1	109/109 (100%)	100 (92%)	9 (8%)	11	39
3	U2	109/109 (100%)	99 (91%)	10 (9%)	9	34
3	U3	109/109 (100%)	96 (88%)	13 (12%)	5	25
3	U4	109/109 (100%)	92 (84%)	17 (16%)	2	17
3	U5	109/109 (100%)	96 (88%)	13 (12%)	5	25
4	W	53/54 (98%)	48 (91%)	5 (9%)	8	33
4	W1	53/54 (98%)	48 (91%)	5 (9%)	8	33
4	W2	53/54 (98%)	44 (83%)	9 (17%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	W3	53/54 (98%)	45 (85%)	8 (15%)	3	18
4	W4	53/54 (98%)	49 (92%)	4 (8%)	13	42
4	W5	53/54 (98%)	43 (81%)	10 (19%)	1	10
4	w	53/54 (98%)	44 (83%)	9 (17%)	2	14
4	w1	53/54 (98%)	48 (91%)	5 (9%)	8	33
4	w2	53/54 (98%)	48 (91%)	5 (9%)	8	33
4	w3	53/54 (98%)	46 (87%)	7 (13%)	4	22
4	w4	53/54 (98%)	49 (92%)	4 (8%)	13	42
4	w5	53/54 (98%)	48 (91%)	5 (9%)	8	33
7	f	91/94 (97%)	79 (87%)	12 (13%)	4	22
7	f1	91/94 (97%)	82 (90%)	9 (10%)	8	31
7	f2	91/94 (97%)	84 (92%)	7 (8%)	13	42
7	f3	91/94 (97%)	79 (87%)	12 (13%)	4	22
7	f4	91/94 (97%)	77 (85%)	14 (15%)	2	17
7	f5	91/94 (97%)	83 (91%)	8 (9%)	10	37
All	All	12192/12882 (95%)	11412 (94%)	780 (6%)	21	47

All (780) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	HIS
1	B	35	LEU
1	B	43	GLU
1	B	54	THR
1	B	76	LEU
1	B	82	VAL
1	B	84	SER
1	B	116	LYS
1	B	123	CYS
1	B	133	THR
1	B	147	PHE
1	B	151	LEU
1	B	156	THR
1	B	166	ARG
1	B	241	GLU
1	B	256	GLU
1	B	262	ASP

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Mol	Chain	Res	Type
1	B	265	GLN
1	B	269	LEU
1	B	273	ILE
1	B	287	ASP
1	B	330	VAL
1	B	337	ASP
1	B	341	LEU
1	B	354	PHE
1	B	369	SER
1	B	379	GLN
1	B	381	SER
1	B	384	THR
1	B	446	ASP
1	B	453	MET
1	B	467	LEU
1	B	478	GLU
2	O	16	THR
2	O	29	ASN
2	O	31	LEU
2	O	59	TYR
2	O	67	TRP
2	O	70	THR
2	O	83	THR
2	O	102	GLU
2	O	104	ASP
2	O	131	VAL
2	O	138	THR
2	O	145	ASN
2	O	155	ARG
2	O	159	THR
2	O	174	VAL
2	O	191	THR
2	O	242	THR
2	P	8	MET
2	P	35	ASP
2	P	46	THR
2	P	67	TRP
2	P	84	LEU
2	P	121	ARG
2	P	155	ARG
2	P	162	THR
2	P	173	VAL

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Mol	Chain	Res	Type
2	P	174	VAL
2	P	183	VAL
2	P	191	THR
2	Q	38	ARG
2	Q	66	ASP
2	Q	67	TRP
2	Q	102	GLU
2	Q	104	ASP
2	Q	118	ASP
2	Q	145	ASN
2	Q	151	MET
2	Q	215	THR
2	R	33	ASP
2	R	145	ASN
2	R	162	THR
2	R	213	THR
2	R	225	ASN
2	R	232	ASN
3	U	30	ARG
3	U	39	PHE
3	U	52	THR
3	U	56	LEU
3	U	87	ARG
3	U	110	TYR
3	U	116	ASP
3	U	117	ASP
3	U	130	ILE
2	V	15	THR
2	V	33	ASP
2	V	66	ASP
2	V	68	THR
2	V	84	LEU
2	V	138	THR
2	V	145	ASN
2	V	155	ARG
2	V	162	THR
2	V	165	THR
2	V	225	ASN
2	V	242	THR
2	V	243	VAL
4	W	22	ARG
4	W	26	VAL

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Mol	Chain	Res	Type
4	W	39	SER
4	W	50	LEU
4	W	53	GLN
7	f	4	PHE
7	f	42	VAL
7	f	47	GLU
7	f	54	GLN
7	f	58	VAL
7	f	69	THR
7	f	72	VAL
7	f	75	LEU
7	f	80	THR
7	f	90	VAL
7	f	102	HIS
7	f	113	VAL
4	w	6	GLU
4	w	14	LEU
4	w	18	MET
4	w	21	LYS
4	w	22	ARG
4	w	25	THR
4	w	34	GLU
4	w	39	SER
4	w	54	THR
1	b	25	HIS
1	b	31	PHE
1	b	35	LEU
1	b	49	LEU
1	b	107	PHE
1	b	127	ASP
1	b	171	MET
1	b	241	GLU
1	b	255	MET
1	b	262	ASP
1	b	282	ILE
1	b	287	ASP
1	b	293	ASP
1	b	296	LEU
1	b	333	LEU
1	b	379	GLN
1	b	453	MET
1	b	456	ASP

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Mol	Chain	Res	Type
1	b	476	GLU
1	b	498	MET
7	f1	4	PHE
7	f1	7	LEU
7	f1	9	ASP
7	f1	17	GLU
7	f1	65	LEU
7	f1	93	VAL
7	f1	102	HIS
7	f1	103	LEU
7	f1	113	VAL
4	W1	27	GLN
4	W1	38	THR
4	W1	39	SER
4	W1	50	LEU
4	W1	53	GLN
4	w1	17	LEU
4	w1	23	VAL
4	w1	25	THR
4	w1	39	SER
4	w1	58	GLN
3	U1	14	LEU
3	U1	20	HIS
3	U1	39	PHE
3	U1	52	THR
3	U1	56	LEU
3	U1	59	ASP
3	U1	91	VAL
3	U1	126	LEU
3	U1	132	TYR
1	B1	25	HIS
1	B1	31	PHE
1	B1	35	LEU
1	B1	72	ASN
1	B1	81	ILE
1	B1	82	VAL
1	B1	91	ARG
1	B1	136	MET
1	B1	154	GLN
1	B1	171	MET
1	B1	202	LEU
1	B1	234	ILE

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Mol	Chain	Res	Type
1	B1	237	PHE
1	B1	241	GLU
1	B1	255	MET
1	B1	257	GLN
1	B1	269	LEU
1	B1	325	LEU
1	B1	330	VAL
1	B1	345	GLN
1	B1	455	ILE
1	B1	456	ASP
1	b1	31	PHE
1	b1	35	LEU
1	b1	82	VAL
1	b1	86	PHE
1	b1	120	GLU
1	b1	124	CYS
1	b1	132	ARG
1	b1	145	HIS
1	b1	218	LYS
1	b1	252	TYR
1	b1	255	MET
1	b1	259	LYS
1	b1	260	MET
1	b1	261	LEU
1	b1	269	LEU
1	b1	273	ILE
1	b1	274	VAL
1	b1	277	MET
1	b1	339	LEU
1	b1	359	LEU
1	b1	370	TYR
1	b1	417	GLU
1	b1	423	ARG
1	b1	453	MET
1	b1	484	ASP
7	f2	4	PHE
7	f2	7	LEU
7	f2	45	ASP
7	f2	58	VAL
7	f2	65	LEU
7	f2	75	LEU
7	f2	113	VAL

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Mol	Chain	Res	Type
4	W2	22	ARG
4	W2	23	VAL
4	W2	25	THR
4	W2	26	VAL
4	W2	27	GLN
4	W2	39	SER
4	W2	45	LYS
4	W2	51	GLU
4	W2	60	ARG
4	w2	19	THR
4	w2	23	VAL
4	w2	29	ASP
4	w2	51	GLU
4	w2	53	GLN
3	U2	4	MET
3	U2	7	THR
3	U2	9	LEU
3	U2	39	PHE
3	U2	52	THR
3	U2	66	HIS
3	U2	74	GLN
3	U2	114	ARG
3	U2	128	TYR
3	U2	134	MET
1	B2	35	LEU
1	B2	125	CYS
1	B2	151	LEU
1	B2	166	ARG
1	B2	167	THR
1	B2	292	MET
1	B2	296	LEU
1	B2	330	VAL
1	B2	334	MET
1	B2	341	LEU
1	B2	384	THR
1	B2	411	MET
1	B2	453	MET
1	B2	467	LEU
1	B2	472	LEU
1	B2	474	THR
1	B2	478	GLU
1	B2	505	LEU

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Mol	Chain	Res	Type
1	b2	31	PHE
1	b2	35	LEU
1	b2	43	GLU
1	b2	67	ASN
1	b2	79	ASP
1	b2	107	PHE
1	b2	132	ARG
1	b2	138	ILE
1	b2	170	ARG
1	b2	171	MET
1	b2	215	MET
1	b2	218	LYS
1	b2	242	ASP
1	b2	259	LYS
1	b2	269	LEU
1	b2	273	ILE
1	b2	359	LEU
1	b2	456	ASP
1	b2	501	ARG
7	f3	4	PHE
7	f3	6	ASN
7	f3	7	LEU
7	f3	49	ILE
7	f3	59	GLU
7	f3	65	LEU
7	f3	75	LEU
7	f3	79	ASP
7	f3	90	VAL
7	f3	103	LEU
7	f3	113	VAL
7	f3	116	ARG
4	W3	16	ASP
4	W3	23	VAL
4	W3	25	THR
4	W3	34	GLU
4	W3	49	GLU
4	W3	50	LEU
4	W3	59	ARG
4	W3	66	PHE
4	w3	16	ASP
4	w3	26	VAL
4	w3	32	ARG

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Mol	Chain	Res	Type
4	w3	36	THR
4	w3	49	GLU
4	w3	50	LEU
4	w3	56	MET
3	U3	19	LYS
3	U3	34	PHE
3	U3	39	PHE
3	U3	52	THR
3	U3	74	GLN
3	U3	77	ASP
3	U3	100	ASP
3	U3	101	LEU
3	U3	126	LEU
3	U3	129	VAL
3	U3	130	ILE
3	U3	132	TYR
3	U3	134	MET
1	B3	25	HIS
1	B3	34	GLN
1	B3	35	LEU
1	B3	43	GLU
1	B3	82	VAL
1	B3	86	PHE
1	B3	132	ARG
1	B3	140	GLU
1	B3	171	MET
1	B3	173	SER
1	B3	179	ASN
1	B3	202	LEU
1	B3	206	VAL
1	B3	215	MET
1	B3	218	LYS
1	B3	225	GLU
1	B3	255	MET
1	B3	274	VAL
1	B3	337	ASP
1	B3	340	ASN
1	B3	380	MET
1	B3	498	MET
1	b3	25	HIS
1	b3	31	PHE
1	b3	35	LEU

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Mol	Chain	Res	Type
1	b3	43	GLU
1	b3	76	LEU
1	b3	82	VAL
1	b3	91	ARG
1	b3	147	PHE
1	b3	171	MET
1	b3	218	LYS
1	b3	255	MET
1	b3	339	LEU
1	b3	379	GLN
1	b3	433	PHE
1	b3	455	ILE
1	b3	474	THR
1	b3	505	LEU
7	f4	4	PHE
7	f4	7	LEU
7	f4	25	THR
7	f4	28	THR
7	f4	30	THR
7	f4	49	ILE
7	f4	58	VAL
7	f4	75	LEU
7	f4	76	ARG
7	f4	86	GLU
7	f4	97	ASP
7	f4	103	LEU
7	f4	113	VAL
7	f4	116	ARG
4	W4	23	VAL
4	W4	39	SER
4	W4	49	GLU
4	W4	51	GLU
4	w4	16	ASP
4	w4	26	VAL
4	w4	50	LEU
4	w4	56	MET
3	U4	17	LEU
3	U4	19	LYS
3	U4	20	HIS
3	U4	30	ARG
3	U4	39	PHE
3	U4	44	VAL

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Mol	Chain	Res	Type
3	U4	52	THR
3	U4	59	ASP
3	U4	64	GLU
3	U4	75	VAL
3	U4	88	ILE
3	U4	91	VAL
3	U4	92	MET
3	U4	117	ASP
3	U4	122	SER
3	U4	130	ILE
3	U4	132	TYR
1	B4	31	PHE
1	B4	35	LEU
1	B4	125	CYS
1	B4	137	MET
1	B4	166	ARG
1	B4	181	ASN
1	B4	237	PHE
1	B4	252	TYR
1	B4	254	VAL
1	B4	255	MET
1	B4	269	LEU
1	B4	292	MET
1	B4	325	LEU
1	B4	330	VAL
1	B4	341	LEU
1	B4	345	GLN
1	B4	358	LEU
1	B4	369	SER
1	B4	370	TYR
1	B4	384	THR
1	B4	413	LEU
1	B4	474	THR
1	B4	487	GLN
1	B4	498	MET
1	b4	31	PHE
1	b4	35	LEU
1	b4	39	ASN
1	b4	77	HIS
1	b4	86	PHE
1	b4	127	ASP
1	b4	172	VAL

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Mol	Chain	Res	Type
1	b4	202	LEU
1	b4	204	TYR
1	b4	237	PHE
1	b4	252	TYR
1	b4	255	MET
1	b4	258	MET
1	b4	262	ASP
1	b4	277	MET
1	b4	286	LEU
1	b4	287	ASP
1	b4	339	LEU
1	b4	345	GLN
1	b4	354	PHE
1	b4	369	SER
1	b4	379	GLN
1	b4	444	ASN
1	b4	453	MET
1	b4	456	ASP
1	b4	474	THR
7	f5	4	PHE
7	f5	28	THR
7	f5	33	GLU
7	f5	49	ILE
7	f5	70	ASP
7	f5	75	LEU
7	f5	86	GLU
7	f5	103	LEU
4	W5	14	LEU
4	W5	17	LEU
4	W5	23	VAL
4	W5	25	THR
4	W5	43	LEU
4	W5	50	LEU
4	W5	52	VAL
4	W5	54	THR
4	W5	56	MET
4	W5	61	ARG
4	w5	2	THR
4	w5	7	LEU
4	w5	14	LEU
4	w5	23	VAL
4	w5	29	ASP

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Mol	Chain	Res	Type
3	U5	4	MET
3	U5	19	LYS
3	U5	20	HIS
3	U5	22	THR
3	U5	30	ARG
3	U5	39	PHE
3	U5	52	THR
3	U5	56	LEU
3	U5	66	HIS
3	U5	75	VAL
3	U5	77	ASP
3	U5	122	SER
3	U5	134	MET
1	B5	31	PHE
1	B5	35	LEU
1	B5	39	ASN
1	B5	49	LEU
1	B5	79	ASP
1	B5	95	ARG
1	B5	193	VAL
1	B5	202	LEU
1	B5	233	PHE
1	B5	255	MET
1	B5	257	GLN
1	B5	258	MET
1	B5	262	ASP
1	B5	283	GLU
1	B5	380	MET
1	B5	450	SER
1	B5	452	ARG
1	B5	466	MET
1	B5	476	GLU
1	B5	498	MET
1	b5	35	LEU
1	b5	43	GLU
1	b5	82	VAL
1	b5	85	PHE
1	b5	122	ASP
1	b5	136	MET
1	b5	153	VAL
1	b5	156	THR
1	b5	171	MET

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Mol	Chain	Res	Type
1	b5	194	GLN
1	b5	202	LEU
1	b5	218	LYS
1	b5	254	VAL
1	b5	258	MET
1	b5	269	LEU
1	b5	273	ILE
1	b5	292	MET
1	b5	296	LEU
1	b5	333	LEU
1	b5	356	GLN
1	b5	371	GLU
1	b5	453	MET
1	b5	474	THR
1	b5	498	MET
2	v	10	VAL
2	v	33	ASP
2	v	57	ASP
2	v	64	ASP
2	v	90	GLU
2	v	105	THR
2	v	148	ARG
2	v	183	VAL
2	v	191	THR
2	V1	16	THR
2	V1	38	ARG
2	V1	39	LEU
2	V1	44	ASP
2	V1	87	MET
2	V1	90	GLU
2	V1	102	GLU
2	V1	131	VAL
2	V1	135	GLU
2	V1	145	ASN
2	V1	174	VAL
2	V1	201	ASP
2	V1	242	THR
2	v1	16	THR
2	v1	19	VAL
2	v1	38	ARG
2	v1	116	THR
2	v1	132	THR

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Mol	Chain	Res	Type
2	v1	135	GLU
2	v1	159	THR
2	v1	162	THR
2	v1	206	THR
2	V2	16	THR
2	V2	35	ASP
2	V2	38	ARG
2	V2	42	VAL
2	V2	119	VAL
2	V2	140	THR
2	V2	155	ARG
2	V2	174	VAL
2	V2	214	ILE
2	V2	215	THR
2	V2	243	VAL
2	v2	62	ASP
2	v2	64	ASP
2	v2	74	GLN
2	v2	75	LYS
2	v2	96	LEU
2	v2	97	LEU
2	v2	104	ASP
2	v2	118	ASP
2	v2	132	THR
2	v2	135	GLU
2	v2	164	MET
2	v2	196	ARG
2	v2	215	THR
2	o	16	THR
2	o	55	TYR
2	o	59	TYR
2	o	62	ASP
2	o	74	GLN
2	o	96	LEU
2	o	105	THR
2	o	162	THR
2	o	180	THR
2	O1	33	ASP
2	O1	35	ASP
2	O1	61	ASP
2	O1	64	ASP
2	O1	67	TRP

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Mol	Chain	Res	Type
2	O1	84	LEU
2	O1	90	GLU
2	O1	96	LEU
2	O1	132	THR
2	O1	145	ASN
2	O1	195	PHE
2	O1	212	MET
2	O1	240	GLU
2	o1	11	LYS
2	o1	16	THR
2	o1	55	TYR
2	o1	56	ASP
2	o1	59	TYR
2	o1	94	GLN
2	o1	137	ILE
2	o1	162	THR
2	o1	196	ARG
2	o1	203	THR
2	o1	225	ASN
2	O2	16	THR
2	O2	39	LEU
2	O2	45	LEU
2	O2	56	ASP
2	O2	59	TYR
2	O2	67	TRP
2	O2	84	LEU
2	O2	102	GLU
2	O2	145	ASN
2	O2	148	ARG
2	O2	155	ARG
2	O2	204	LYS
2	o2	11	LYS
2	o2	16	THR
2	o2	44	ASP
2	o2	59	TYR
2	o2	84	LEU
2	o2	96	LEU
2	o2	127	ILE
2	o2	157	THR
2	o2	162	THR
2	o2	232	ASN
2	p	7	THR

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Mol	Chain	Res	Type
2	p	8	MET
2	p	51	THR
2	p	67	TRP
2	p	72	GLN
2	p	120	PHE
2	p	154	ASP
2	p	196	ARG
2	P1	8	MET
2	P1	45	LEU
2	P1	49	GLU
2	P1	67	TRP
2	P1	119	VAL
2	P1	155	ARG
2	P1	174	VAL
2	P1	185	PHE
2	P1	196	ARG
2	P1	232	ASN
2	p1	42	VAL
2	p1	45	LEU
2	p1	60	LEU
2	p1	62	ASP
2	p1	67	TRP
2	p1	162	THR
2	p1	183	VAL
2	p1	192	ASP
2	p1	195	PHE
2	p1	196	ARG
2	p1	217	ASN
2	p1	232	ASN
2	P2	38	ARG
2	P2	62	ASP
2	P2	91	GLN
2	P2	96	LEU
2	P2	164	MET
2	P2	174	VAL
2	P2	191	THR
2	p2	10	VAL
2	p2	16	THR
2	p2	21	LYS
2	p2	38	ARG
2	p2	62	ASP
2	p2	137	ILE

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Mol	Chain	Res	Type
2	p2	142	LYS
2	p2	154	ASP
2	p2	191	THR
2	p2	196	ARG
2	q	35	ASP
2	q	51	THR
2	q	70	THR
2	q	74	GLN
2	q	82	PHE
2	q	84	LEU
2	q	87	MET
2	q	97	LEU
2	q	111	ARG
2	q	162	THR
2	q	196	ARG
2	Q1	29	ASN
2	Q1	64	ASP
2	Q1	67	TRP
2	Q1	148	ARG
2	Q1	155	ARG
2	Q1	193	LYS
2	Q1	215	THR
2	Q1	232	ASN
2	q1	11	LYS
2	q1	51	THR
2	q1	59	TYR
2	q1	102	GLU
2	q1	110	ILE
2	q1	148	ARG
2	q1	162	THR
2	q1	201	ASP
2	Q2	15	THR
2	Q2	16	THR
2	Q2	31	LEU
2	Q2	33	ASP
2	Q2	45	LEU
2	Q2	53	GLU
2	Q2	67	TRP
2	Q2	97	LEU
2	Q2	102	GLU
2	Q2	155	ARG
2	Q2	174	VAL

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Mol	Chain	Res	Type
2	Q2	190	VAL
2	Q2	204	LYS
2	Q2	242	THR
2	q2	16	THR
2	q2	31	LEU
2	q2	70	THR
2	q2	97	LEU
2	q2	162	THR
2	q2	195	PHE
2	q2	241	ILE
2	r	8	MET
2	r	21	LYS
2	r	43	LYS
2	r	79	ASP
2	r	87	MET
2	r	162	THR
2	r	164	MET
2	r	192	ASP
2	R1	67	TRP
2	R1	87	MET
2	R1	90	GLU
2	R1	155	ARG
2	R1	204	LYS
2	R1	212	MET
2	R1	232	ASN
2	R1	235	PHE
2	r1	15	THR
2	r1	16	THR
2	r1	21	LYS
2	r1	41	LYS
2	r1	110	ILE
2	r1	162	THR
2	r1	193	LYS
2	r1	196	ARG
2	r1	228	VAL
2	R2	29	ASN
2	R2	59	TYR
2	R2	70	THR
2	R2	87	MET
2	R2	155	ARG
2	R2	174	VAL
2	R2	232	ASN

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Mol	Chain	Res	Type
2	r2	8	MET
2	r2	87	MET
2	r2	96	LEU
2	r2	116	THR
2	r2	146	VAL
2	r2	162	THR
2	r2	164	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	52	ASN
1	B	66	ASN
1	B	75	GLN
1	B	257	GLN
1	B	379	GLN
2	O	29	ASN
2	O	93	GLN
2	P	5	ASN
2	P	29	ASN
2	Q	93	GLN
2	R	5	ASN
2	R	72	GLN
2	R	186	GLN
3	U	62	GLN
2	V	217	ASN
4	w	4	GLN
1	b	52	ASN
1	b	265	GLN
1	b	492	GLN
3	U1	62	GLN
1	B1	25	HIS
1	B1	217	GLN
1	B1	265	GLN
1	B1	301	GLN
1	B1	345	GLN
1	B1	349	ASN
1	b1	34	GLN
1	b1	39	ASN
1	b1	66	ASN
1	b1	257	GLN

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Mol	Chain	Res	Type
1	b1	492	GLN
7	f2	114	ASN
3	U2	6	HIS
3	U2	20	HIS
1	B2	25	HIS
1	B2	52	ASN
1	B2	148	ASN
1	B2	349	ASN
1	b2	299	ASN
1	b2	332	HIS
1	b2	349	ASN
1	B3	265	GLN
1	B3	301	GLN
1	B3	372	GLN
1	B3	407	GLN
1	b3	66	ASN
1	b3	372	GLN
1	B4	265	GLN
1	B4	345	GLN
1	b4	78	GLN
1	b4	444	ASN
4	W5	4	GLN
4	W5	53	GLN
1	B5	75	GLN
1	B5	257	GLN
1	B5	301	GLN
1	B5	342	GLN
1	b5	270	GLN
1	b5	289	GLN
1	b5	299	ASN
1	b5	301	GLN
1	b5	345	GLN
1	b5	379	GLN
2	v	114	ASN
2	v	177	GLN
2	v	186	GLN
2	v1	72	GLN
2	v2	101	ASN
2	v2	145	ASN
2	o1	94	GLN
2	O2	91	GLN
2	P1	72	GLN

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Mol	Chain	Res	Type
2	P1	177	GLN
2	p1	101	ASN
2	P2	91	GLN
2	P2	101	ASN
2	q	72	GLN
2	Q1	217	ASN
2	Q2	72	GLN
2	Q2	93	GLN
2	r1	72	GLN
2	r1	94	GLN
2	R2	91	GLN
2	R2	93	GLN
2	R2	94	GLN
2	r2	72	GLN
2	r2	177	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 monosaccharides 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.

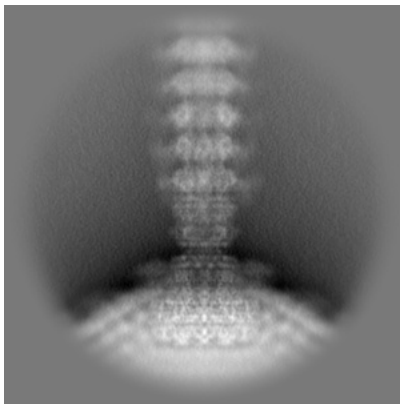
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38556. These allow visual inspection of the internal detail of the map and identification of artifacts.

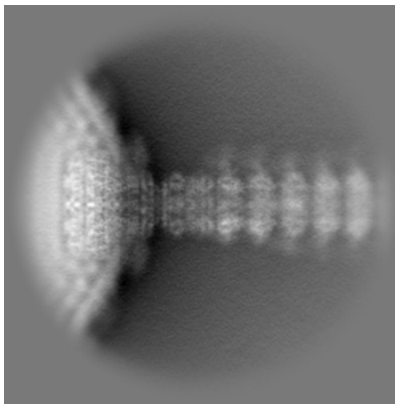
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

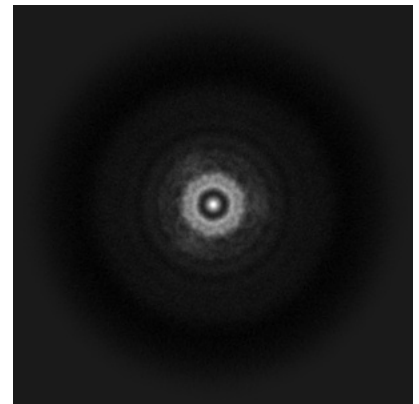
6.1.1 Primary map



X

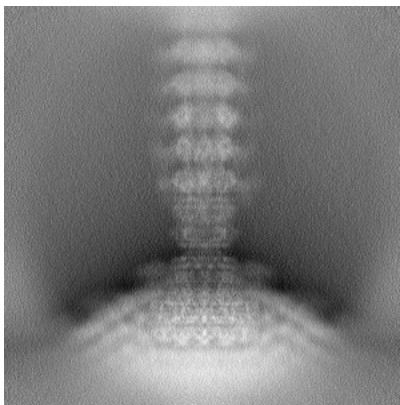


Y

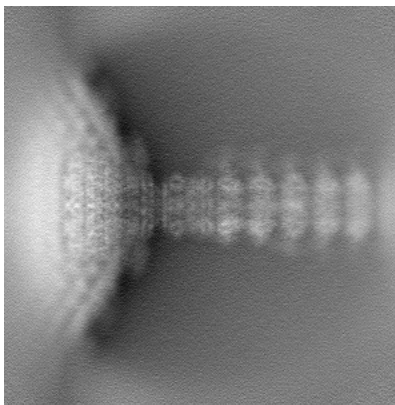


Z

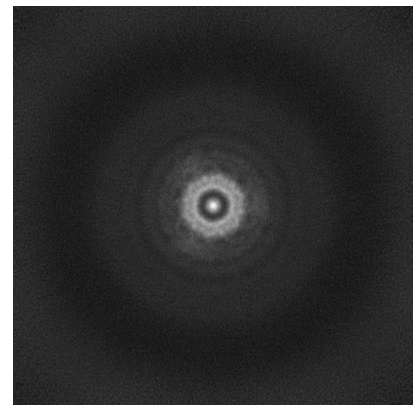
6.1.2 Raw map



X



Y

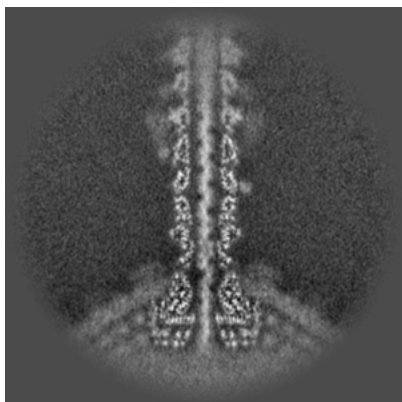


Z

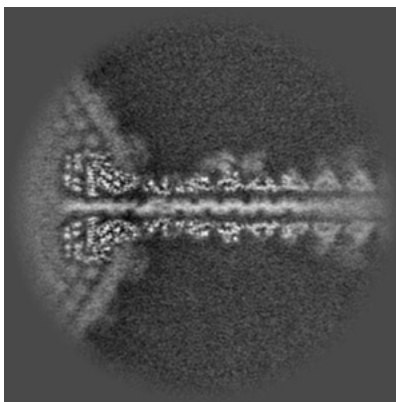
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

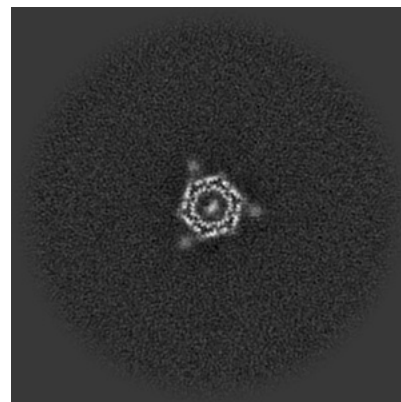
6.2.1 Primary map



X Index: 240

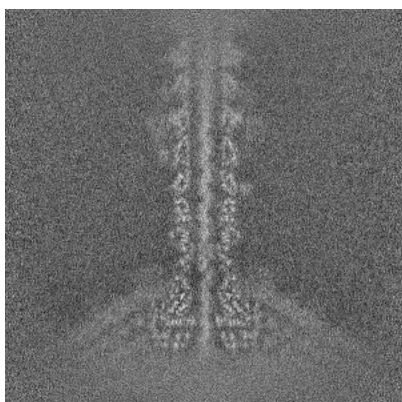


Y Index: 240

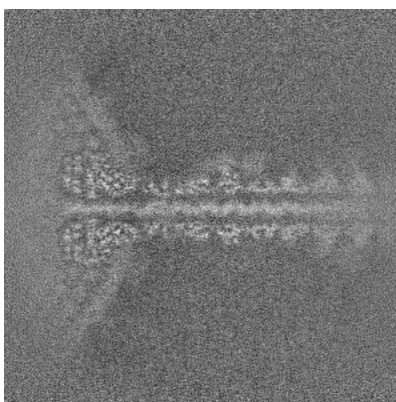


Z Index: 240

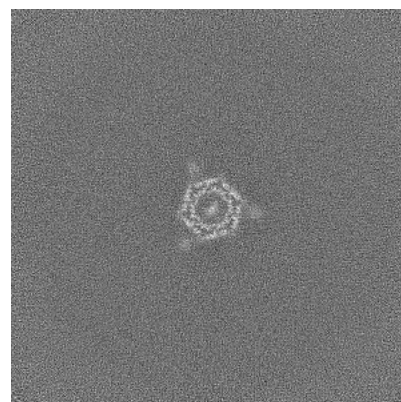
6.2.2 Raw map



X Index: 240



Y Index: 240

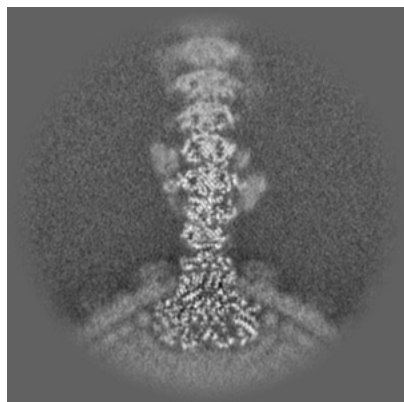


Z Index: 240

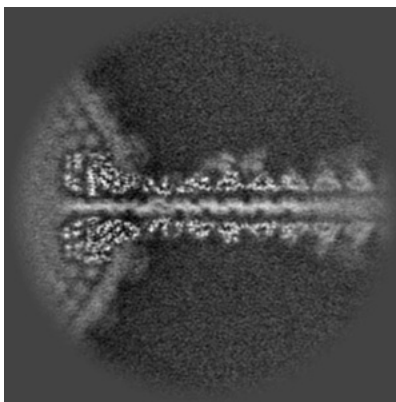
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

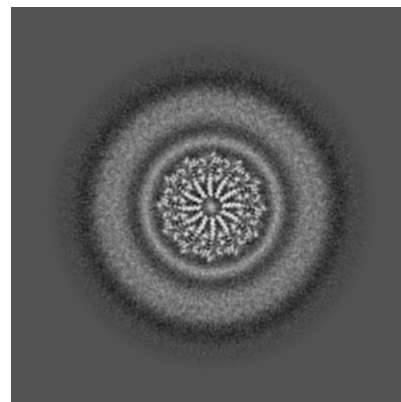
6.3.1 Primary map



X Index: 218

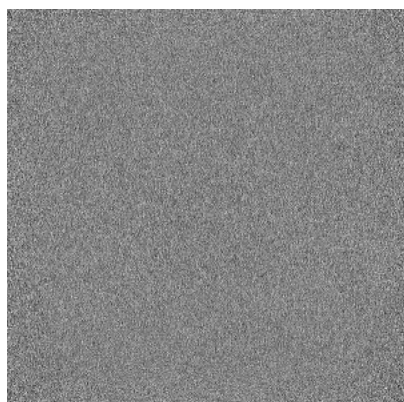


Y Index: 241

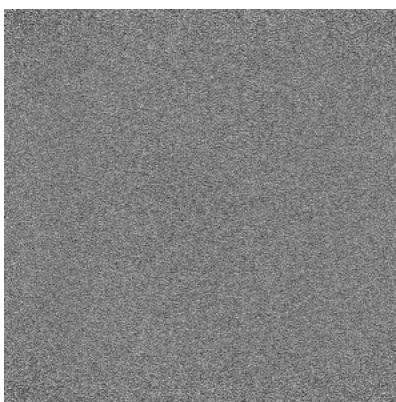


Z Index: 106

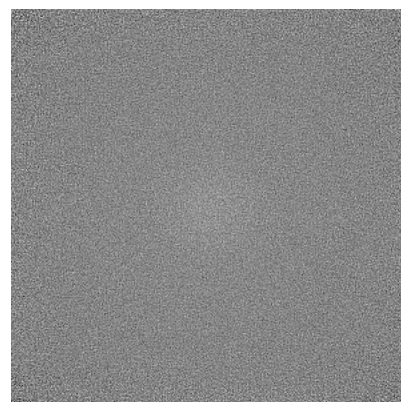
6.3.2 Raw map



X Index: 0



Y Index: 0

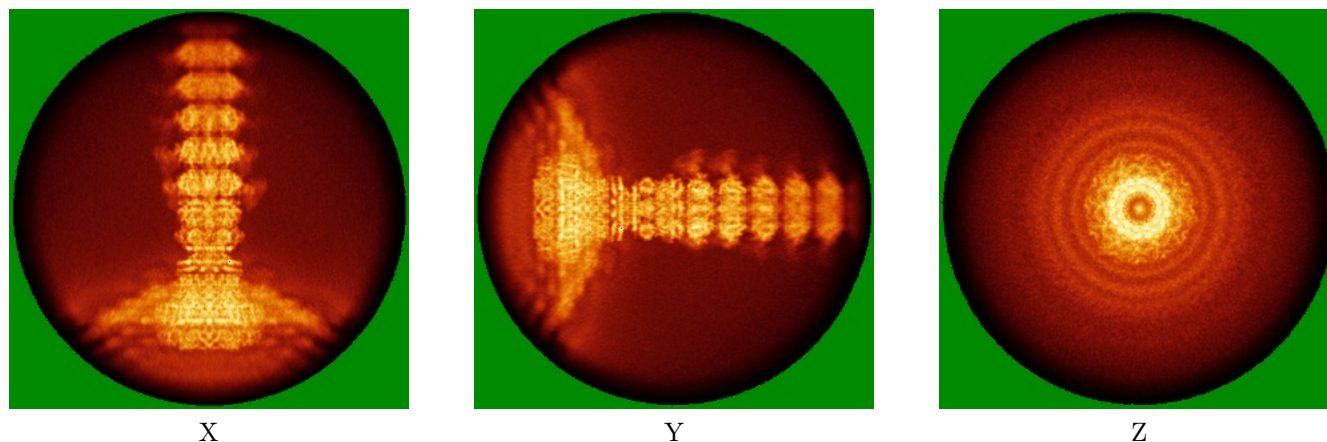


Z Index: 0

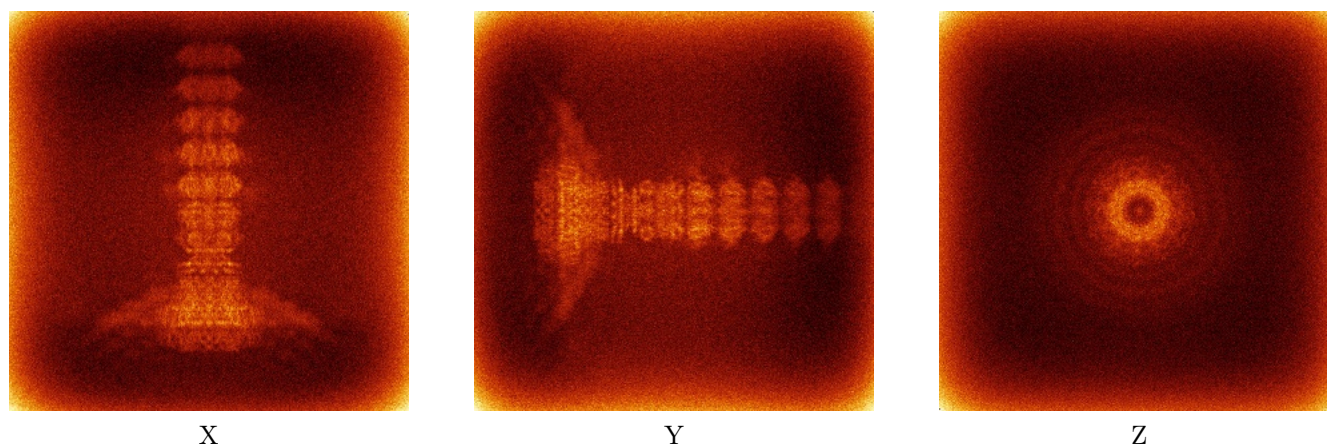
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



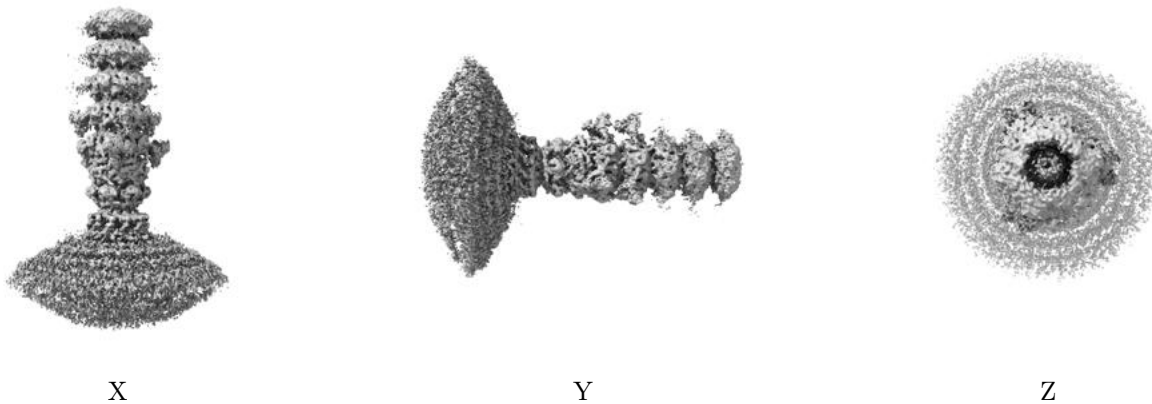
6.4.2 Raw map



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.

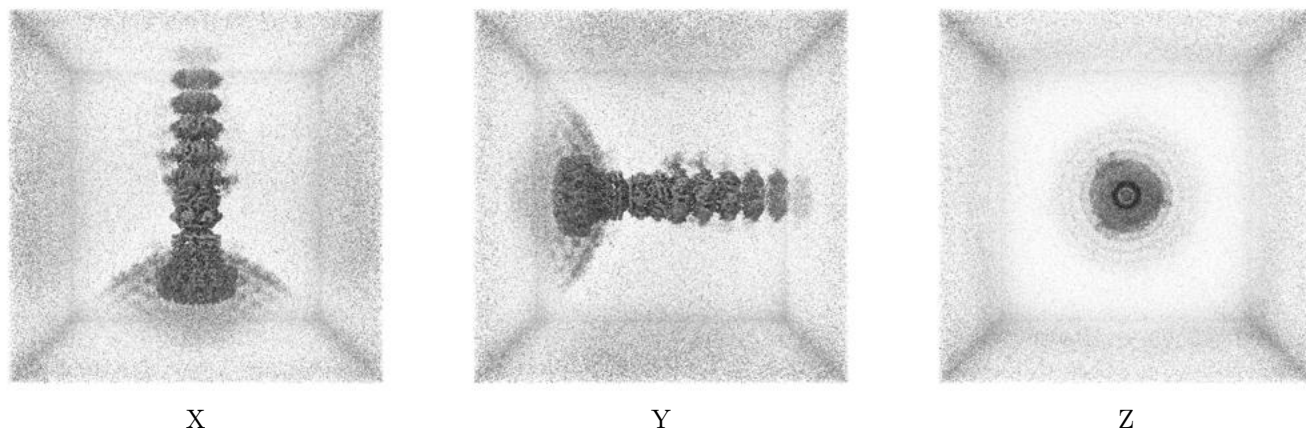
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.52. 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.

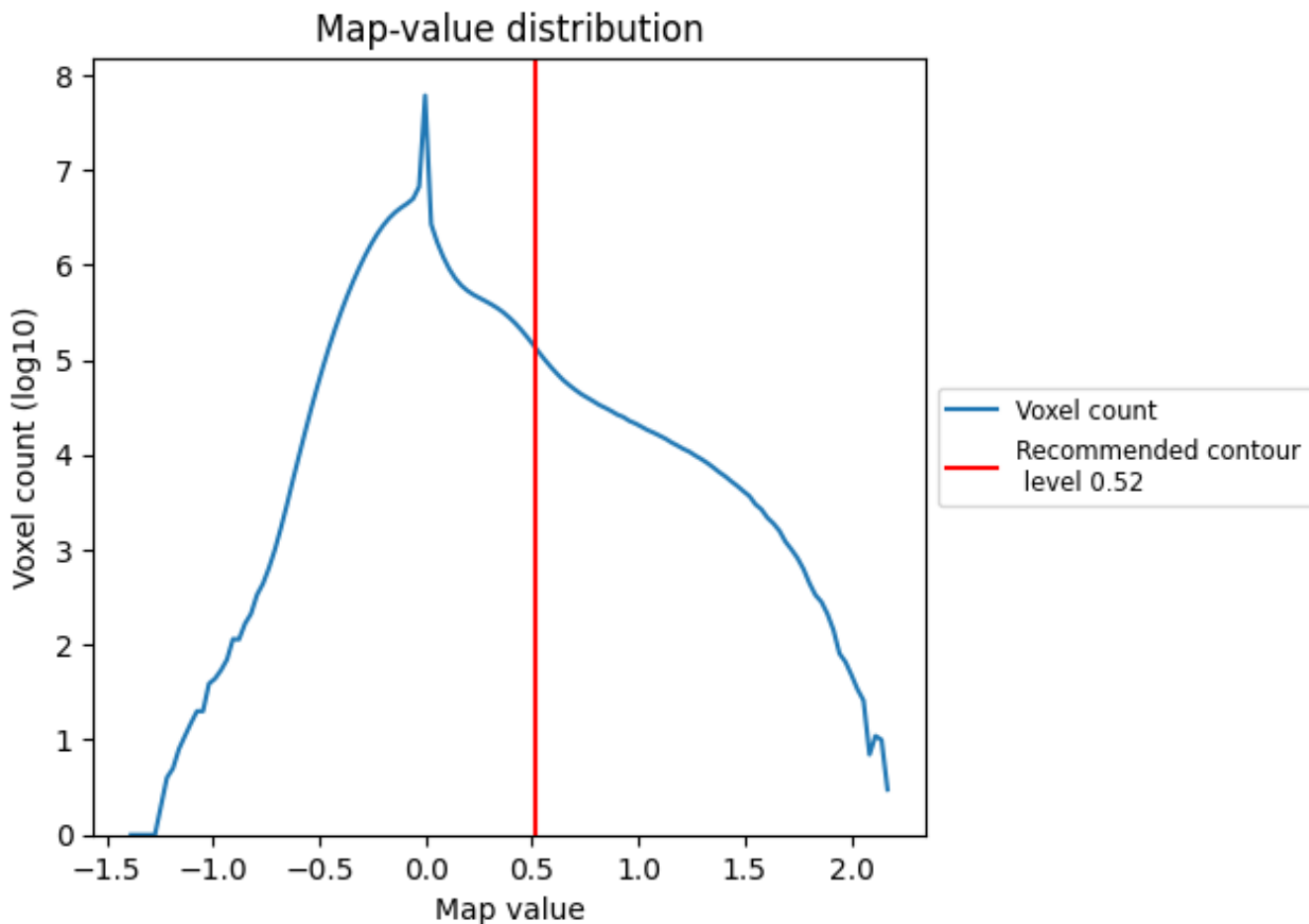
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

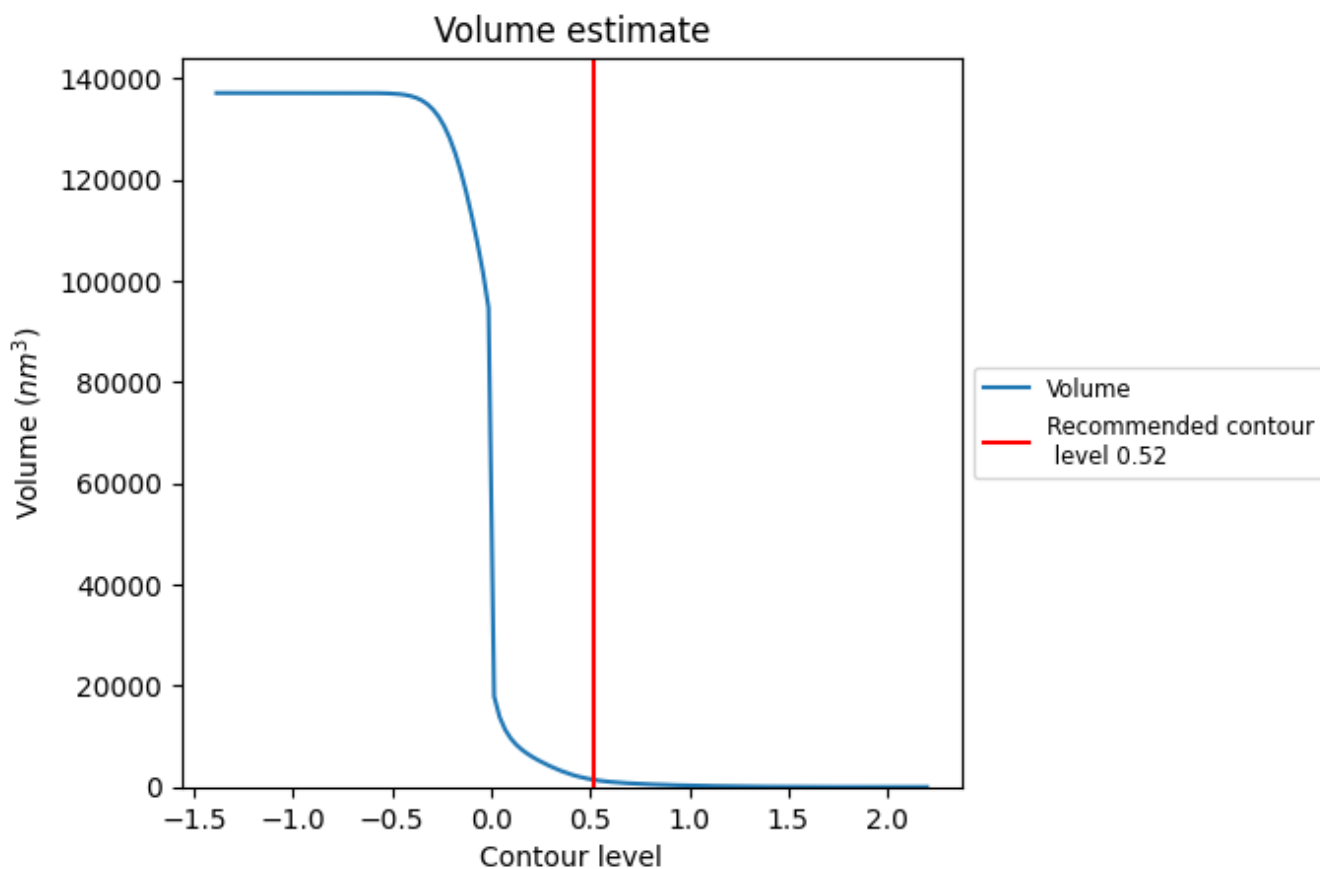
This section contains the results of statistical analysis of the map.

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.

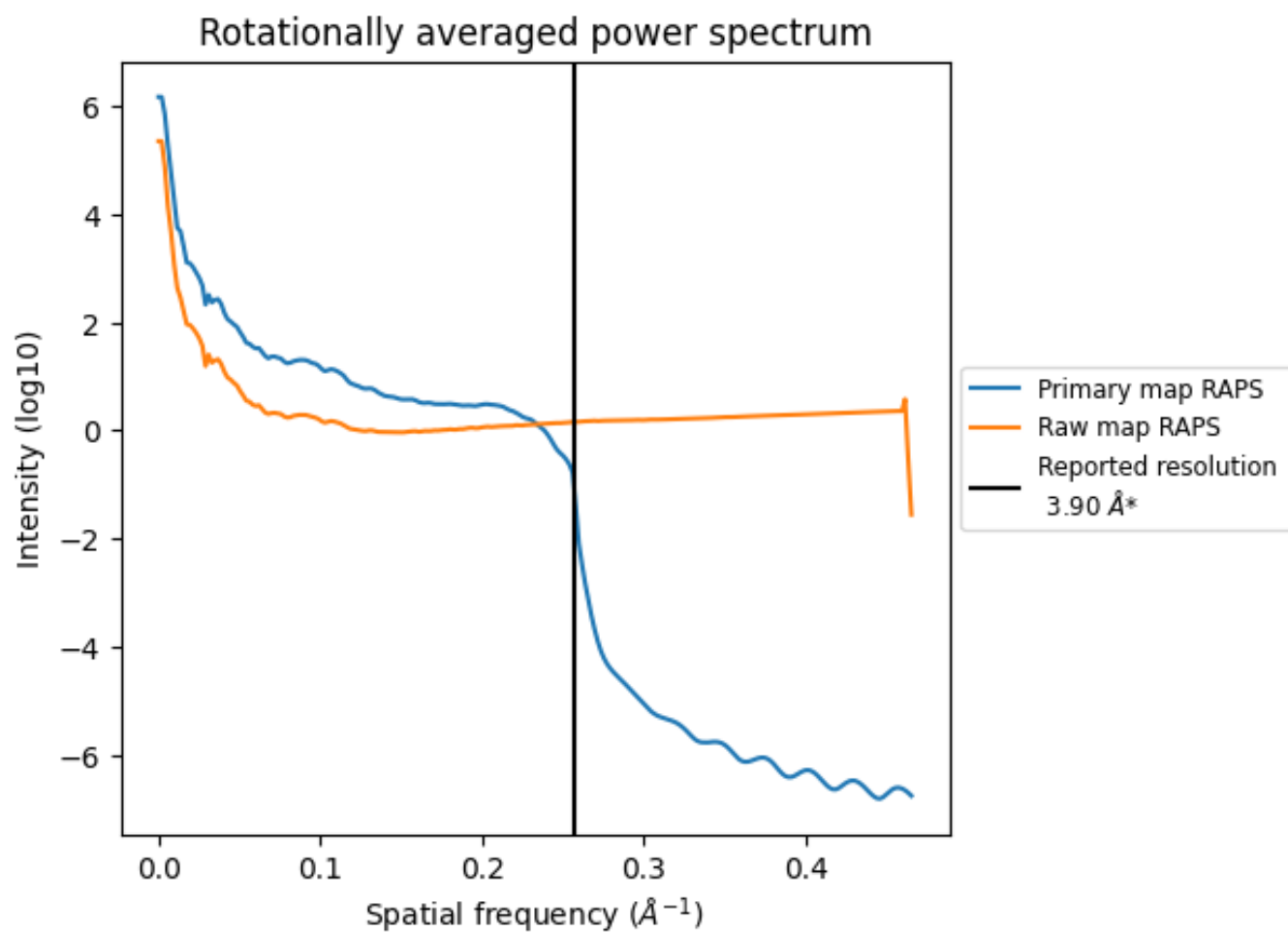
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1400 nm³; this corresponds to an approximate mass of 1265 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 i

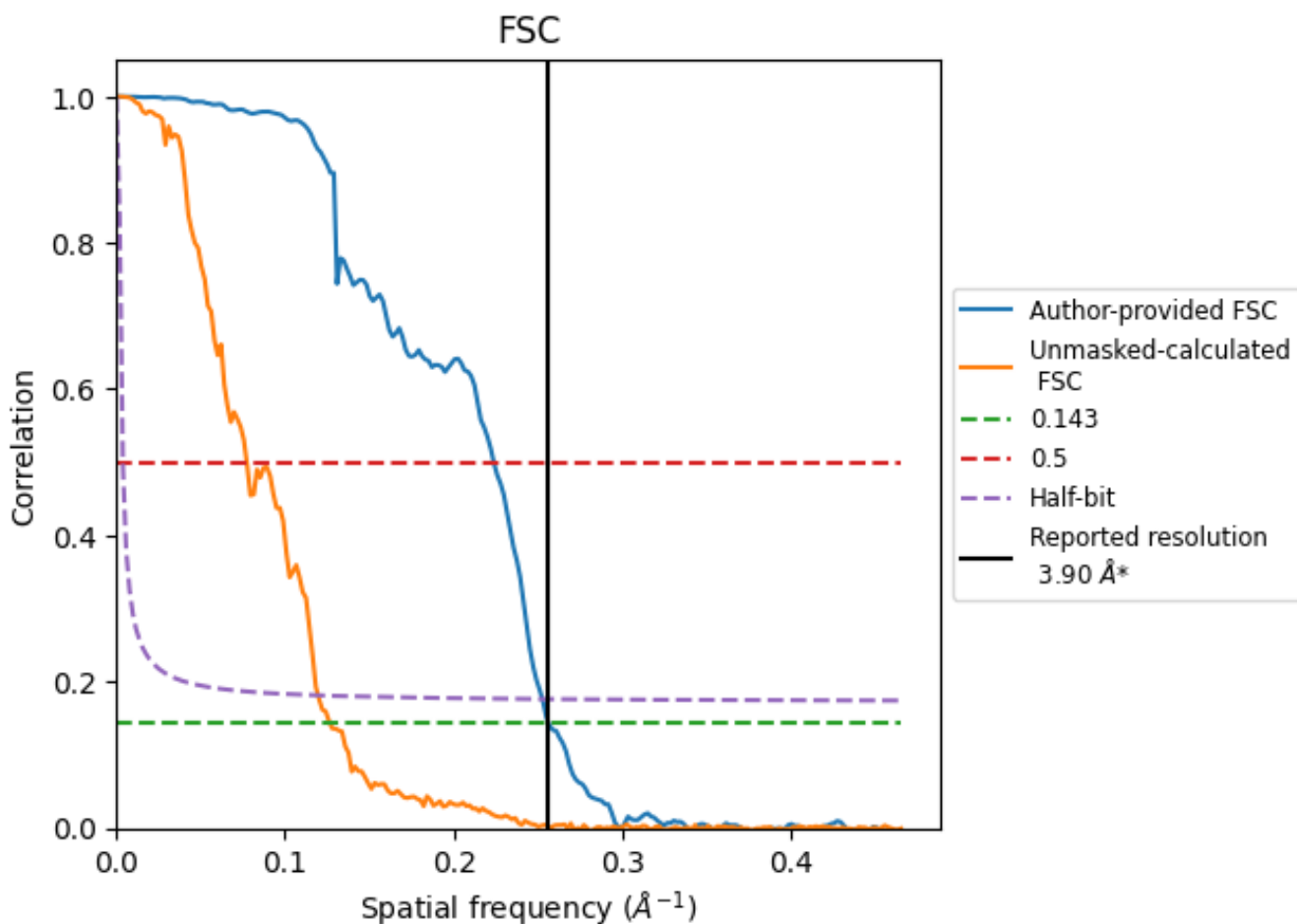


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

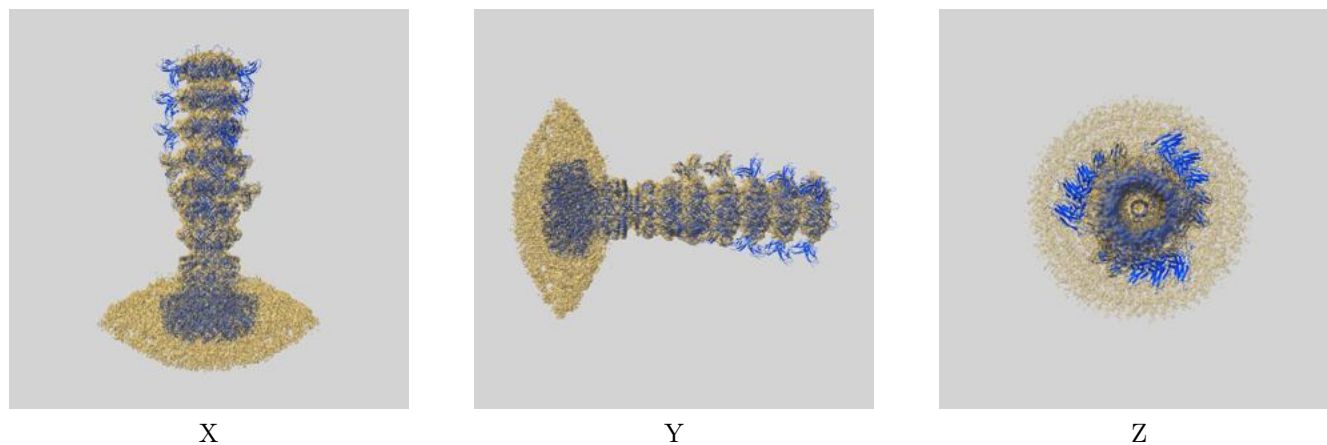
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	4.47	3.96
Unmasked-calculated*	7.90	12.94	8.35

*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 7.90 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

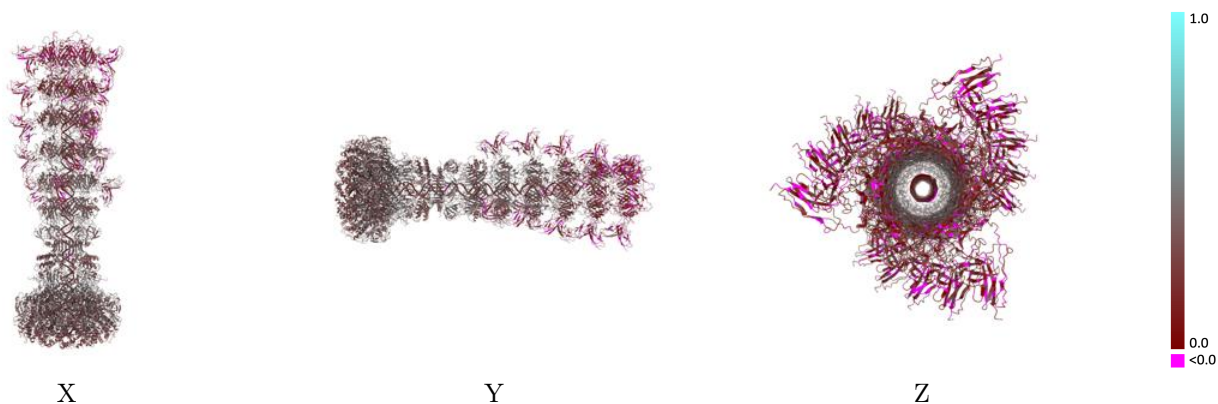
This section contains information regarding the fit between EMDB map EMD-38556 and PDB model 8XPM. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



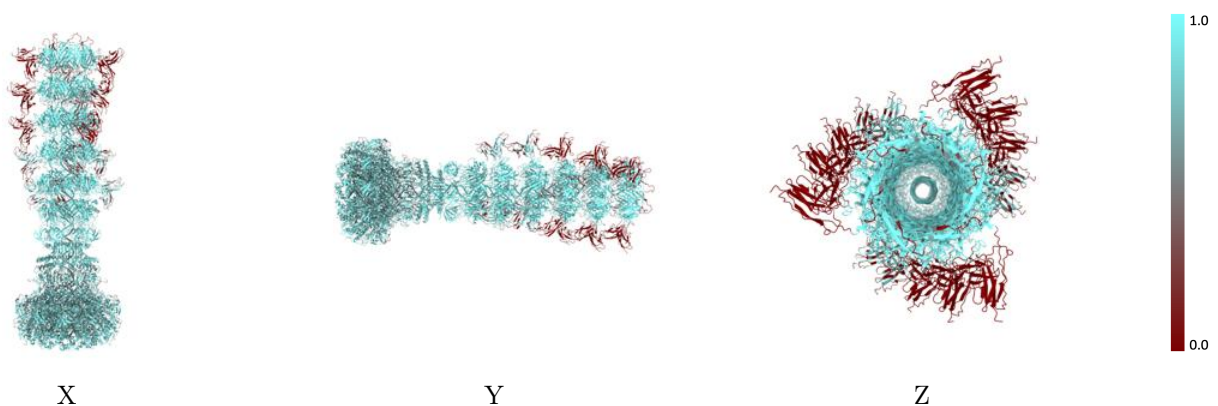
The images above show the 3D surface view of the map at the recommended contour level 0.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



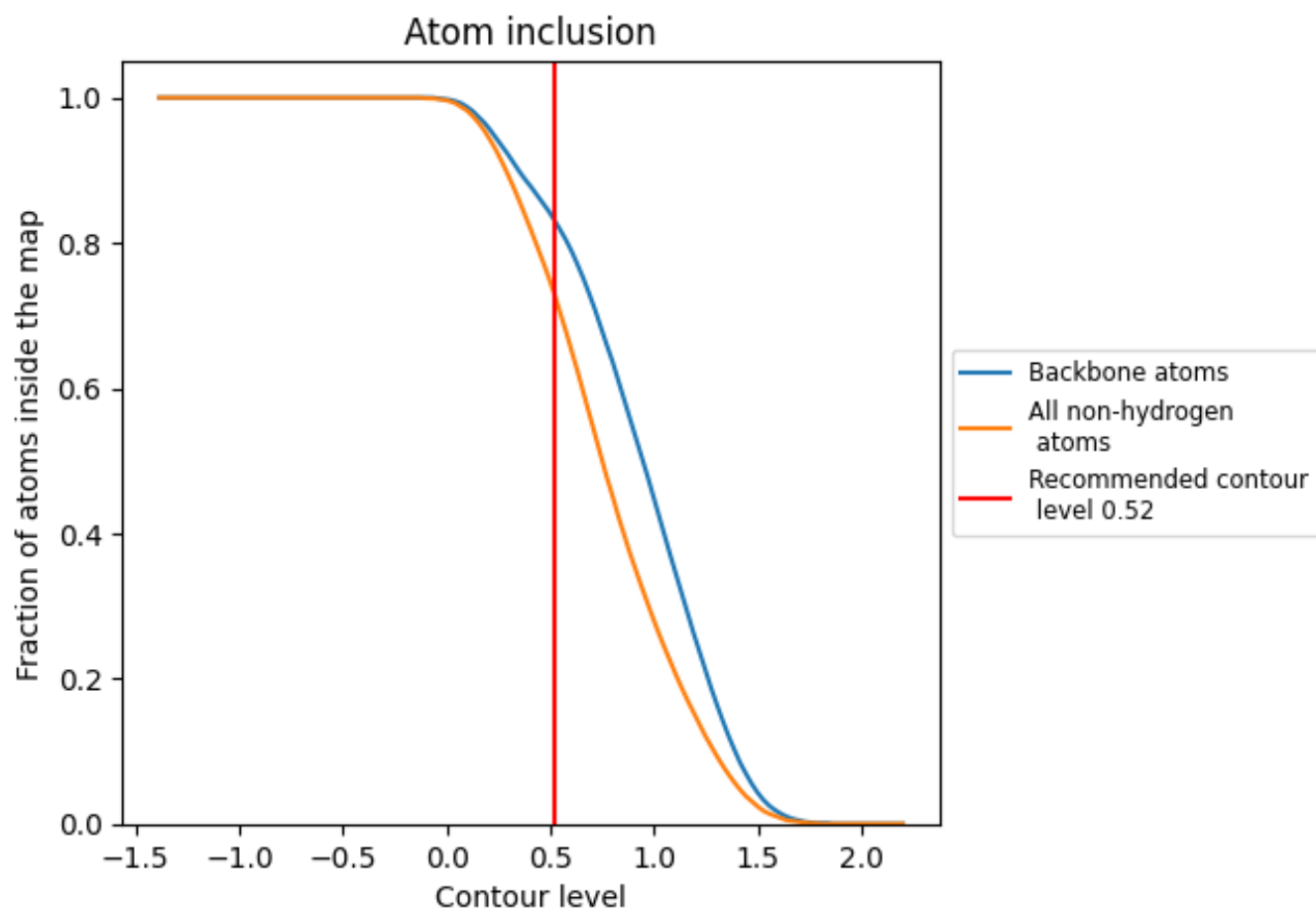
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.52).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 73% 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 (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.3100
B	 0.7540	 0.3630
B1	 0.7580	 0.3640
B2	 0.7550	 0.3690
B3	 0.7630	 0.3710
B4	 0.7660	 0.3690
B5	 0.7470	 0.3660
DA	 0.7530	 0.1910
DB	 0.7500	 0.1890
O	 0.7830	 0.3220
O1	 0.7880	 0.3060
O2	 0.7940	 0.3130
P	 0.6030	 0.2470
P1	 0.6120	 0.2430
P2	 0.6040	 0.2590
Q	 0.5860	 0.1770
Q1	 0.5980	 0.2090
Q2	 0.5900	 0.1930
R	 0.5270	 0.1480
R1	 0.5450	 0.1470
R2	 0.5380	 0.1690
U	 0.8750	 0.3730
U1	 0.8900	 0.3760
U2	 0.8870	 0.3780
U3	 0.8950	 0.3700
U4	 0.9020	 0.3780
U5	 0.8920	 0.3650
V	 0.8150	 0.3240
V1	 0.8180	 0.3320
V2	 0.8360	 0.3500
W	 0.7900	 0.3780
W1	 0.7980	 0.3780
W2	 0.8000	 0.3800
W3	 0.8120	 0.3750
W4	 0.7790	 0.3780



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Chain	Atom inclusion	Q-score
W5	 0.8060	 0.3700
b	 0.7550	 0.3660
b1	 0.7610	 0.3710
b2	 0.7620	 0.3690
b3	 0.7540	 0.3660
b4	 0.7620	 0.3690
b5	 0.7560	 0.3710
f	 0.9000	 0.3970
f1	 0.9020	 0.3940
f2	 0.9020	 0.4010
f3	 0.8910	 0.3920
f4	 0.8960	 0.3900
f5	 0.8930	 0.3850
o	 0.7290	 0.2920
o1	 0.7390	 0.3060
o2	 0.7590	 0.2930
p	 0.6020	 0.2400
p1	 0.6100	 0.2590
p2	 0.6050	 0.2350
q	 0.5810	 0.2050
q1	 0.5730	 0.1920
q2	 0.5780	 0.1960
r	 0.5360	 0.1410
r1	 0.5340	 0.1590
r2	 0.5410	 0.1560
v	 0.7860	 0.3320
v1	 0.8000	 0.3270
v2	 0.8100	 0.3330
w	 0.7770	 0.3680
w1	 0.8020	 0.3770
w2	 0.8260	 0.3740
w3	 0.7900	 0.3790
w4	 0.7980	 0.3710
w5	 0.8000	 0.3750