



Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 10:12 AM EDT

PDB ID : 6WQ2
EMDB ID : EMD-21868
Title : Cryo-EM of the S. islandicus filamentous virus, SIFV
Authors : Wang, F.; Baquero, D.P.; Su, Z.; Zheng, W.; Prangishvili, D.; Krupovic, M.; Egelman, E.H.
Deposited on : 2020-04-28
Resolution : 4.00 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:

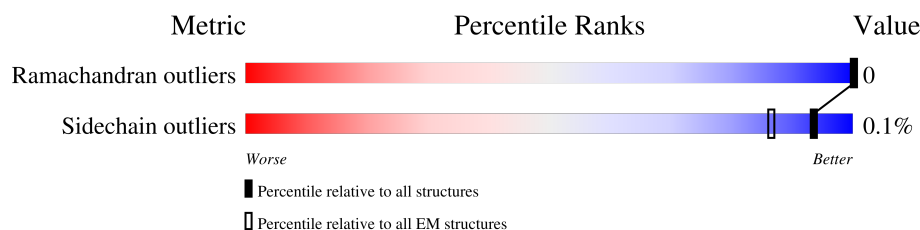
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 4.00 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	1	225	91% 9%
2	2	223	89% 11%
3	A	167	32% 92% 8%
3	B	167	31% 92% 8%
3	C	167	31% 92% 8%
3	D	167	32% 92% 8%
3	E	167	31% 92% 8%
3	F	167	29% 92% 8%
3	G	167	35% 92% 8%

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Mol	Chain	Length	Quality of chain
3	H	167	<div> <div>30%</div> <div>92%</div> <div>8%</div> </div>
3	I	167	<div> <div>30%</div> <div>92%</div> <div>8%</div> </div>
3	J	167	<div> <div>29%</div> <div>92%</div> <div>8%</div> </div>
3	K	167	<div> <div>34%</div> <div>92%</div> <div>8%</div> </div>
3	L	167	<div> <div>32%</div> <div>92%</div> <div>8%</div> </div>
3	M	167	<div> <div>31%</div> <div>92%</div> <div>8%</div> </div>
3	N	167	<div> <div>30%</div> <div>92%</div> <div>8%</div> </div>
3	P	167	<div> <div>35%</div> <div>92%</div> <div>8%</div> </div>
3	R	167	<div> <div>32%</div> <div>92%</div> <div>8%</div> </div>
3	T	167	<div> <div>32%</div> <div>92%</div> <div>8%</div> </div>
4	a	204	<div> <div>38%</div> <div>99%</div> <div>.</div> </div>
4	b	204	<div> <div>37%</div> <div>99%</div> <div>.</div> </div>
4	c	204	<div> <div>37%</div> <div>99%</div> <div>.</div> </div>
4	d	204	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>
4	e	204	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>
4	f	204	<div> <div>37%</div> <div>99%</div> <div>.</div> </div>
4	g	204	<div> <div>37%</div> <div>99%</div> <div>.</div> </div>
4	h	204	<div> <div>37%</div> <div>99%</div> <div>.</div> </div>
4	i	204	<div> <div>37%</div> <div>99%</div> <div>.</div> </div>
4	j	204	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>
4	k	204	<div> <div>38%</div> <div>99%</div> <div>.</div> </div>
4	l	204	<div> <div>37%</div> <div>99%</div> <div>.</div> </div>
4	m	204	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>
4	n	204	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>
4	p	204	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	r	204	<div><div>38%</div><div>99%</div><div>.</div></div>
4	t	204	<div><div>38%</div><div>99%</div><div>.</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 56240 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 DNA chain called A-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	225	Total	C	N	O	P	0	0
			4613	2250	789	1349	225		

- Molecule 2 is a DNA chain called A-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	223	Total	C	N	O	P	0	0
			4571	2230	779	1339	223		

- Molecule 3 is a protein called Structural protein MCP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	B	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	C	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	D	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	E	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	F	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	G	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	H	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	I	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	J	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	K	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	M	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	N	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	P	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	R	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		
3	T	154	Total	C	N	O	S	0	0
			1219	790	202	222	5		

- Molecule 4 is a protein called Structural protein MCP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	b	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	c	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	d	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	e	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	f	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	g	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	h	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	i	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	j	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	k	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	l	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	m	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	p	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	r	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		
4	t	202	Total	C	N	O	S	0	0
			1549	991	255	296	7		

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: A-DNA

Chain 1:  91% 9%



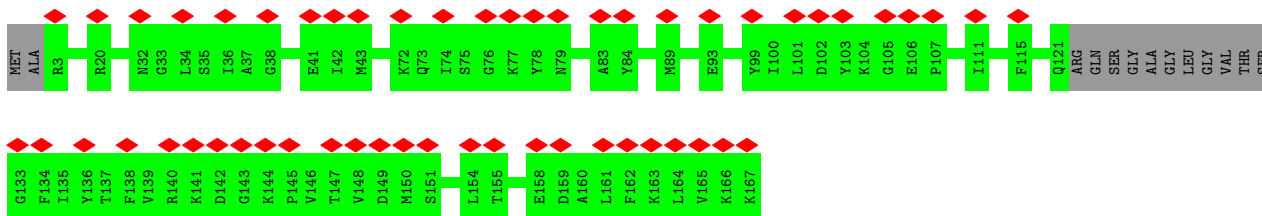
- Molecule 2: A-DNA

Chain 2:  89% 11%



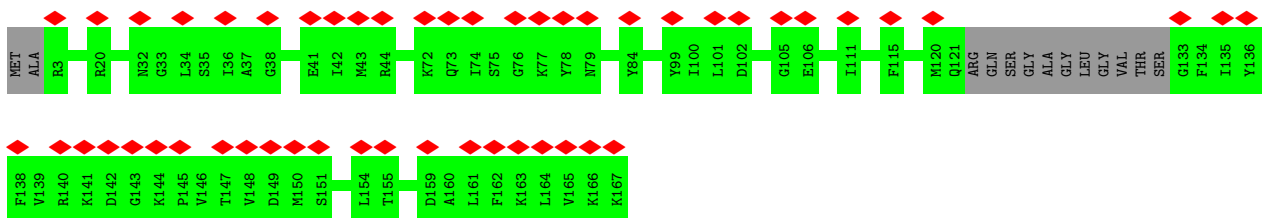
- Molecule 3: Structural protein MCP2

Chain A:  32% 92% 8%

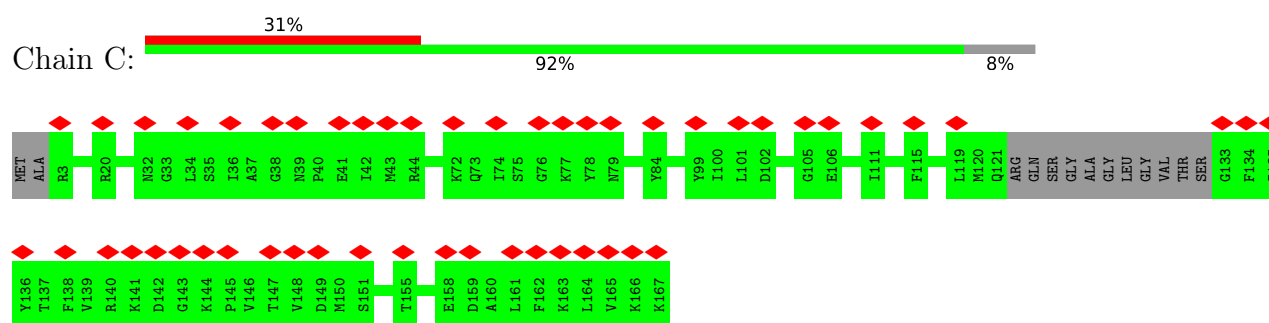


- Molecule 3: Structural protein MCP2

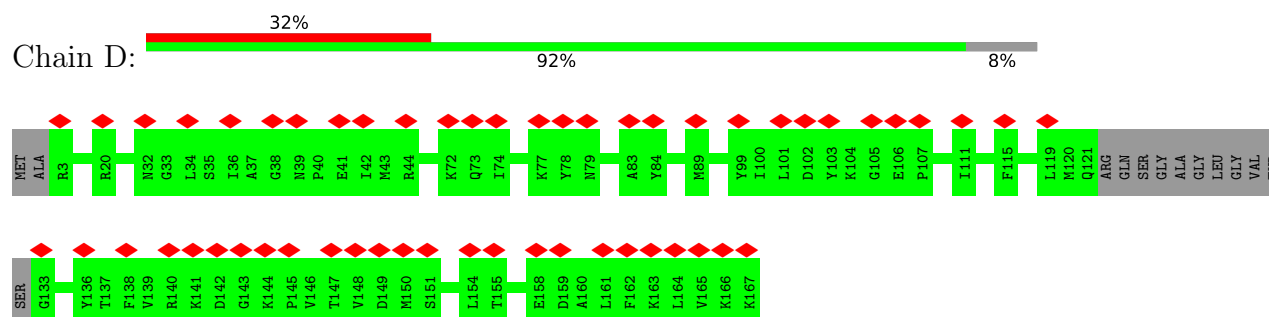
Chain B:  31% 92% 8%



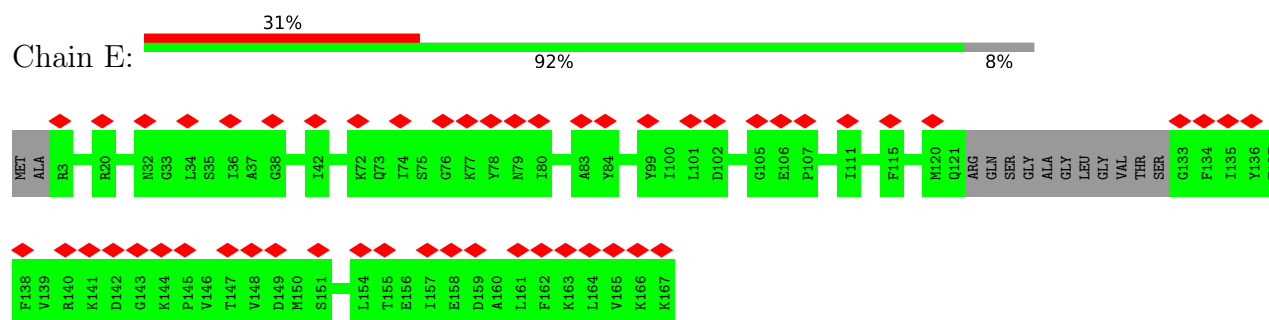
- Molecule 3: Structural protein MCP2



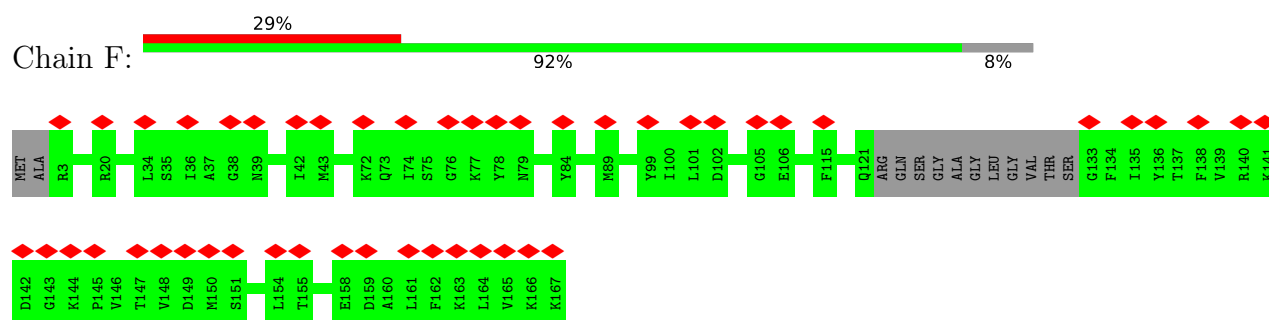
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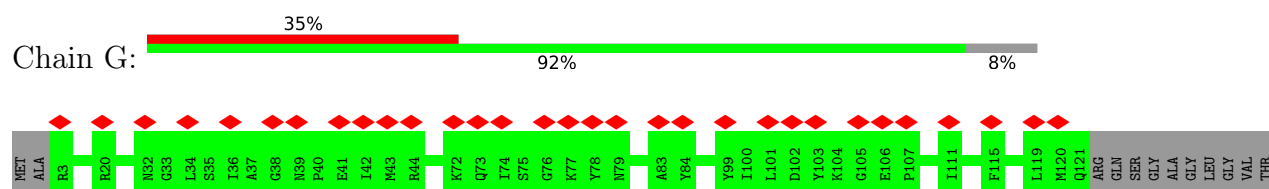
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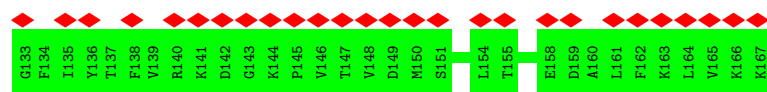


• Molecule 3: Structural protein MCP2

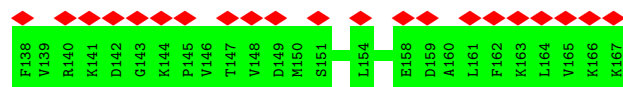
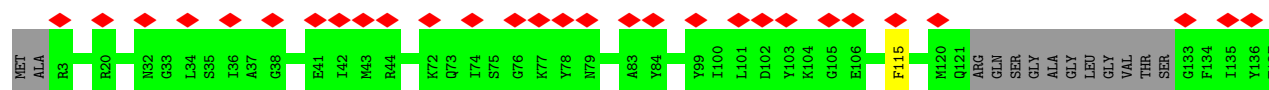
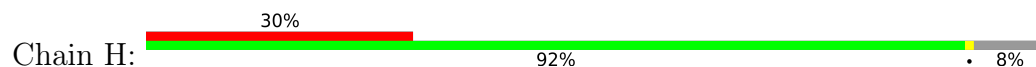


• Molecule 3: Structural protein MCP2

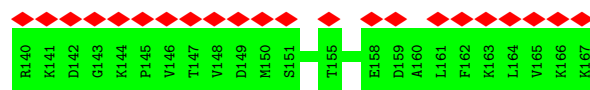
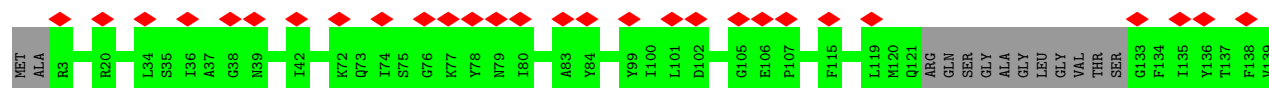




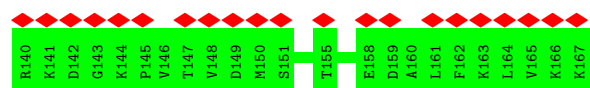
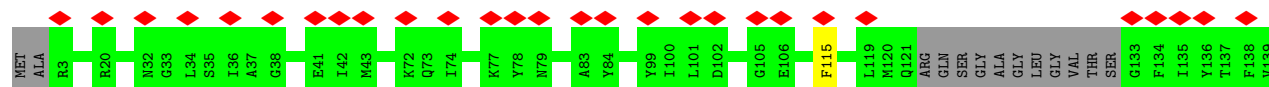
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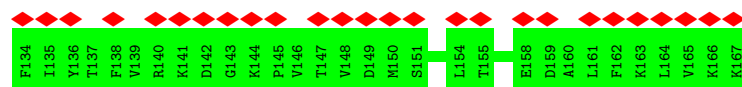
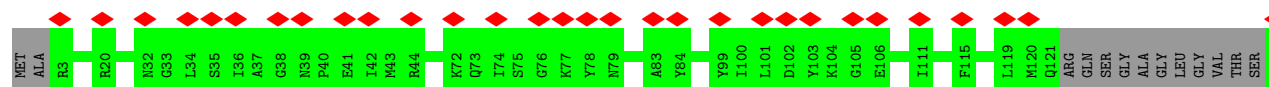
• Molecule 3: Structural protein MCP2



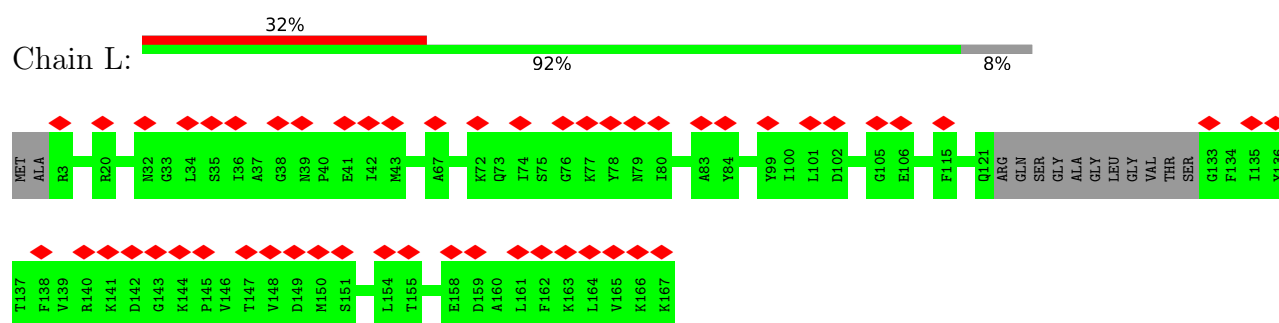
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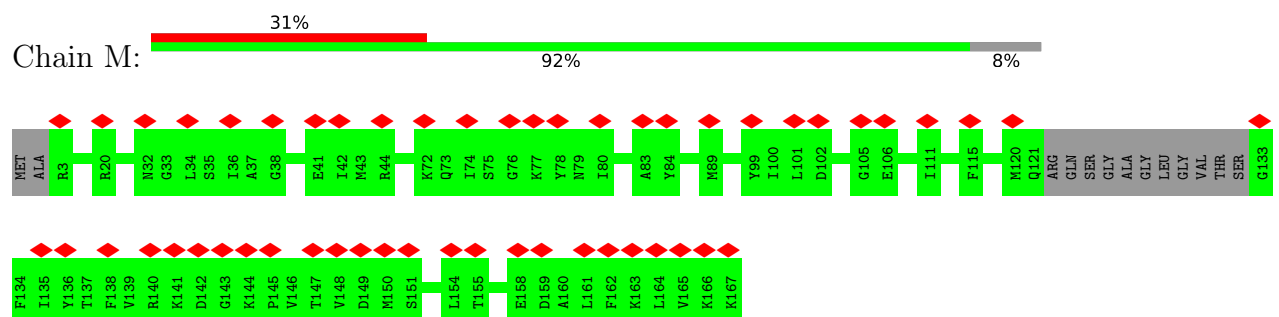
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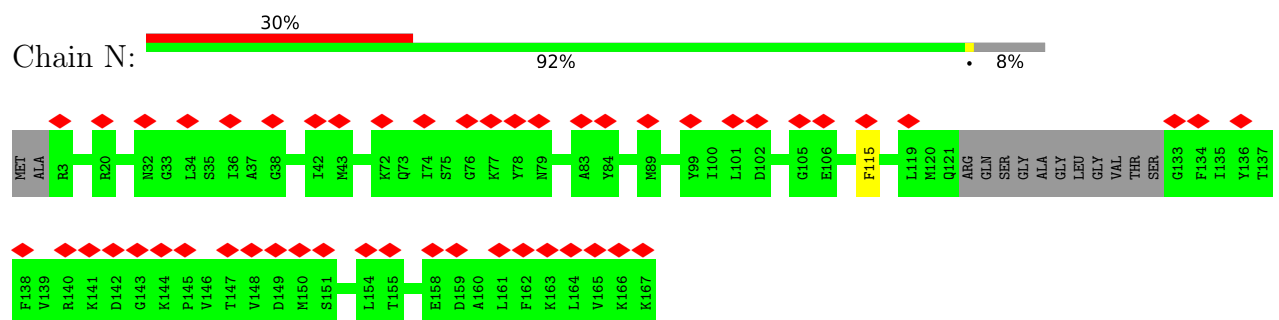
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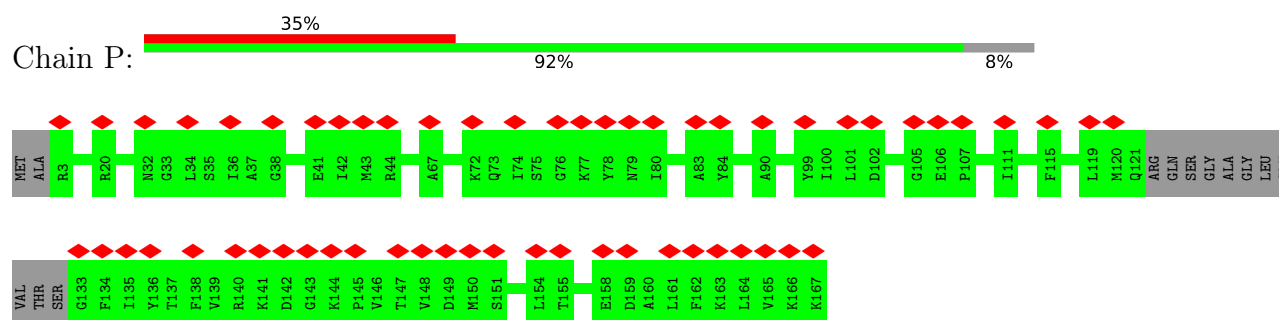
• Molecule 3: Structural protein MCP2



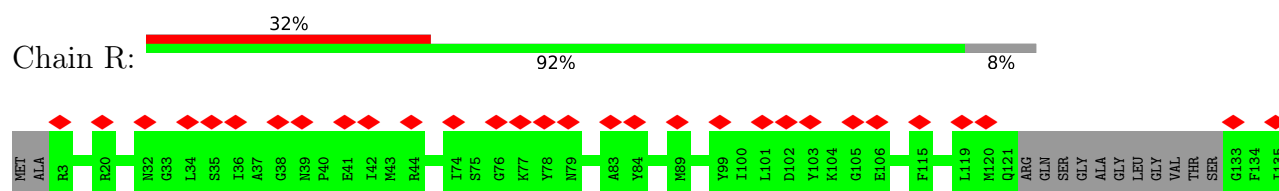
• Molecule 3: Structural protein MCP2

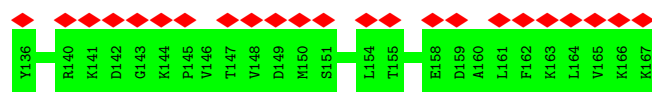


• Molecule 3: Structural protein MCP2

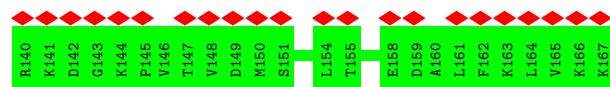
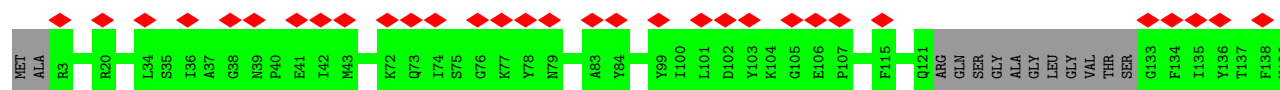


• Molecule 3: Structural protein MCP2

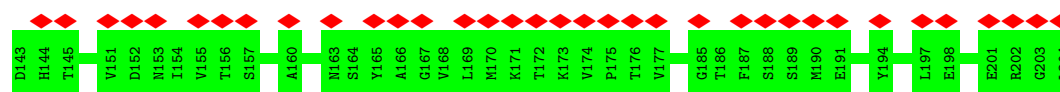
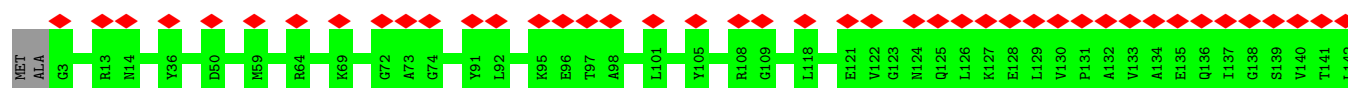
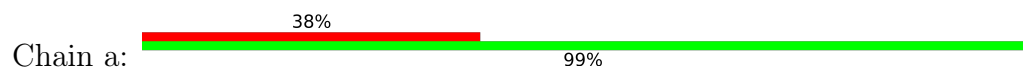




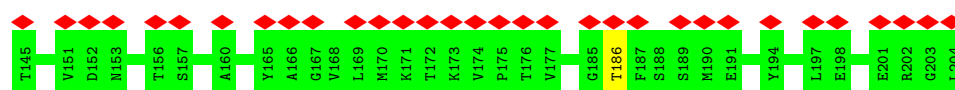
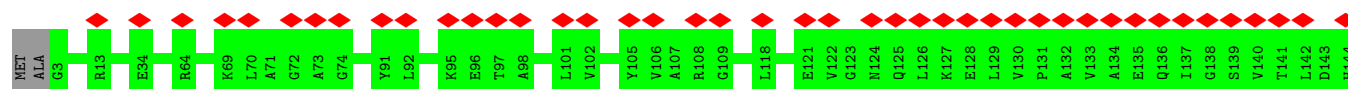
• Molecule 3: Structural protein MCP2



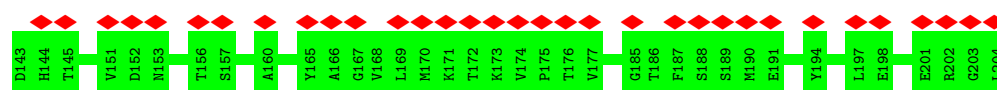
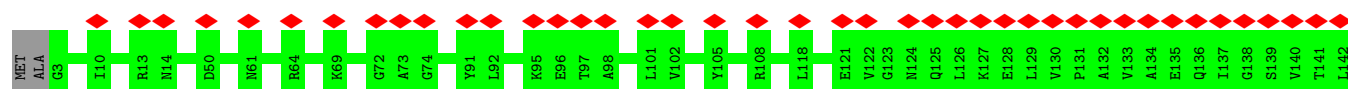
• Molecule 4: Structural protein MCP1



• Molecule 4: Structural protein MCP1

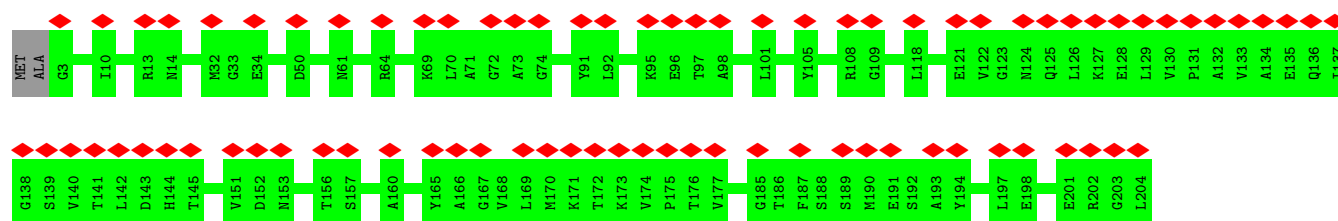


• Molecule 4: Structural protein MCP1



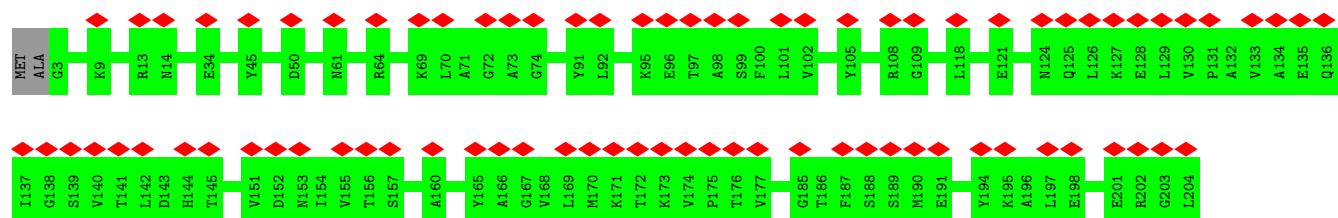
• Molecule 4: Structural protein MCP1

Chain d: 



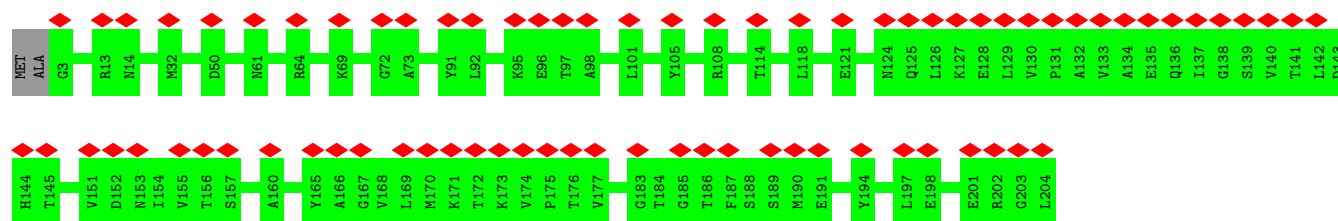
• Molecule 4: Structural protein MCP1

Chain e: 



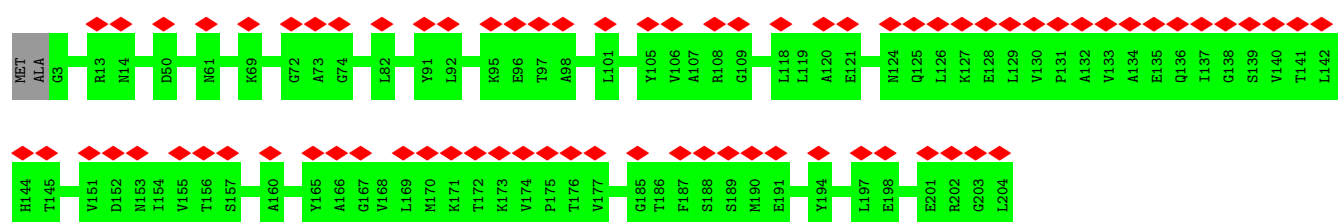
• Molecule 4: Structural protein MCP1

Chain f: 



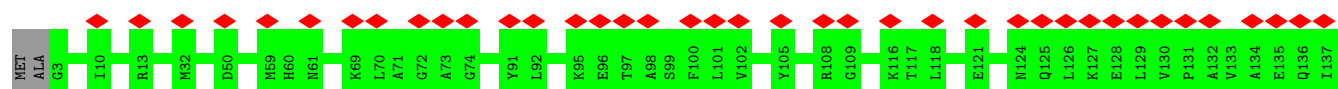
• Molecule 4: Structural protein MCP1

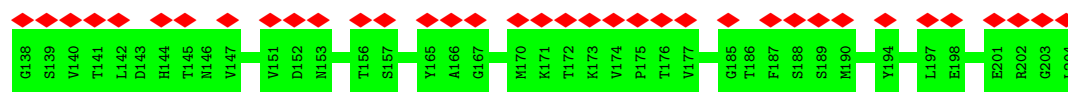
Chain g: 



• Molecule 4: Structural protein MCP1

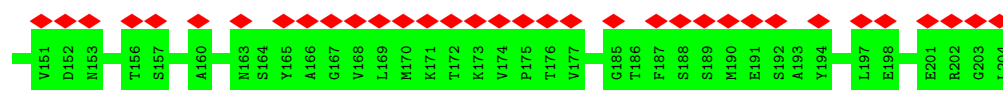
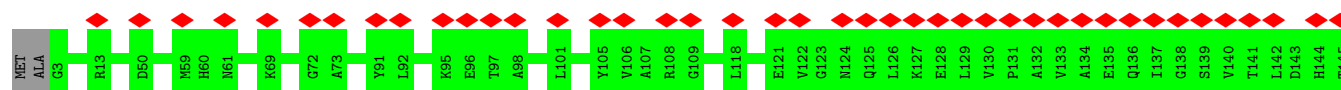
Chain h: 





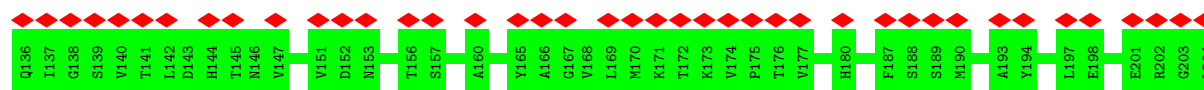
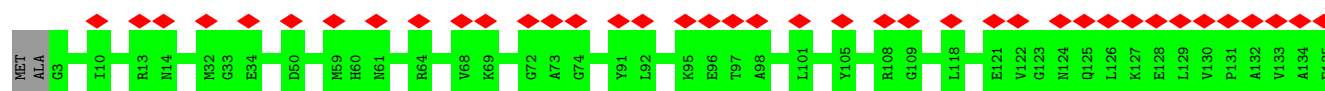
• Molecule 4: Structural protein MCP1

Chain i: 37% 99%



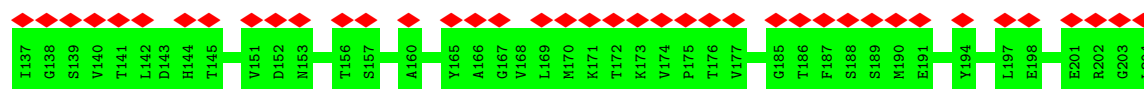
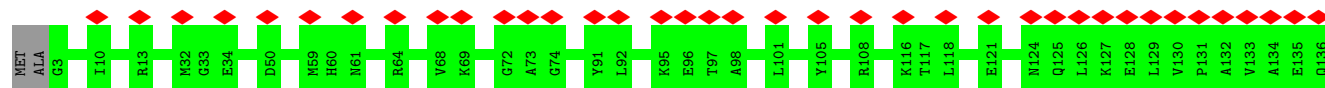
• Molecule 4: Structural protein MCP1

Chain j: 39% 99%



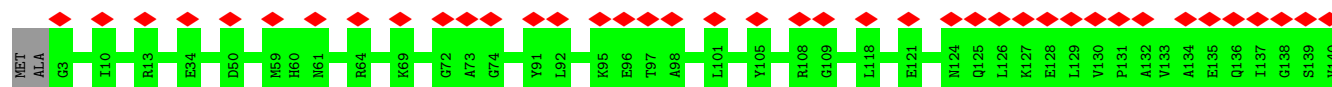
• Molecule 4: Structural protein MCP1

Chain k: 38% 99%

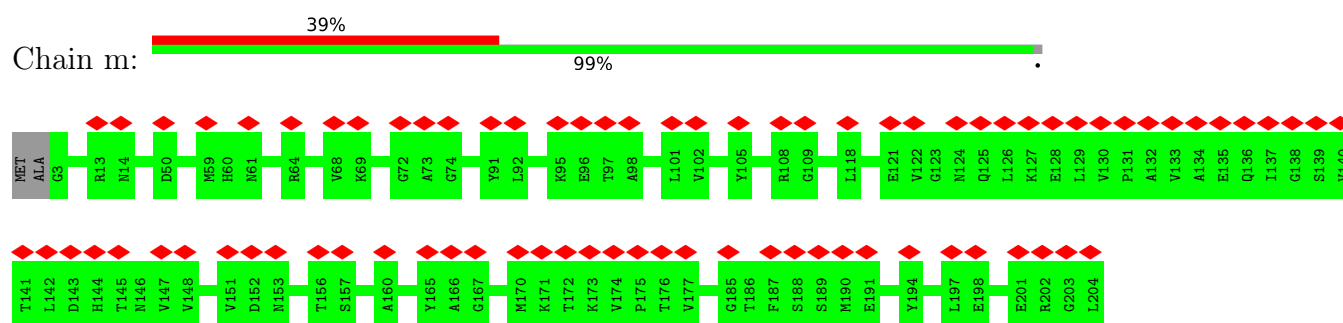


• Molecule 4: Structural protein MCP1

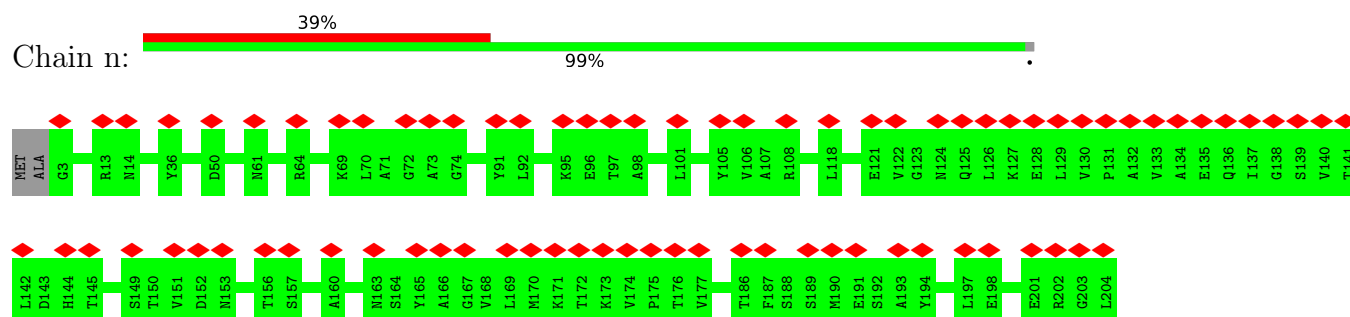
Chain l: 37% 99%



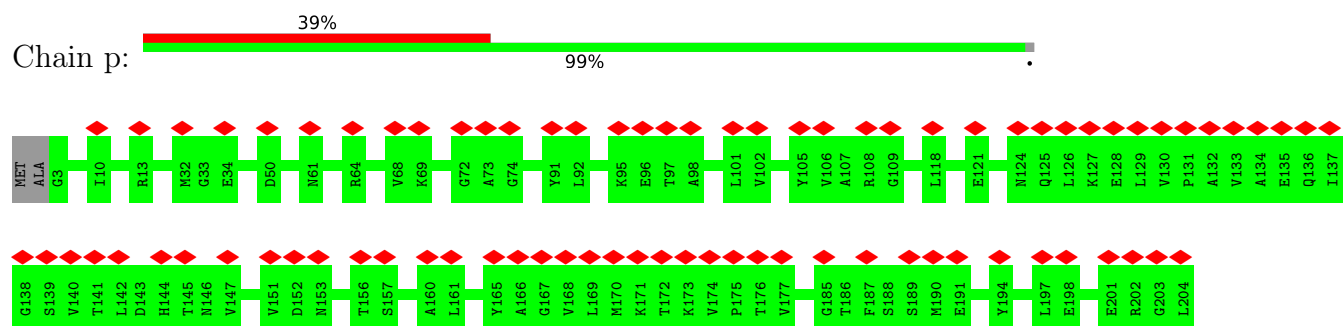
• Molecule 4: Structural protein MCP1



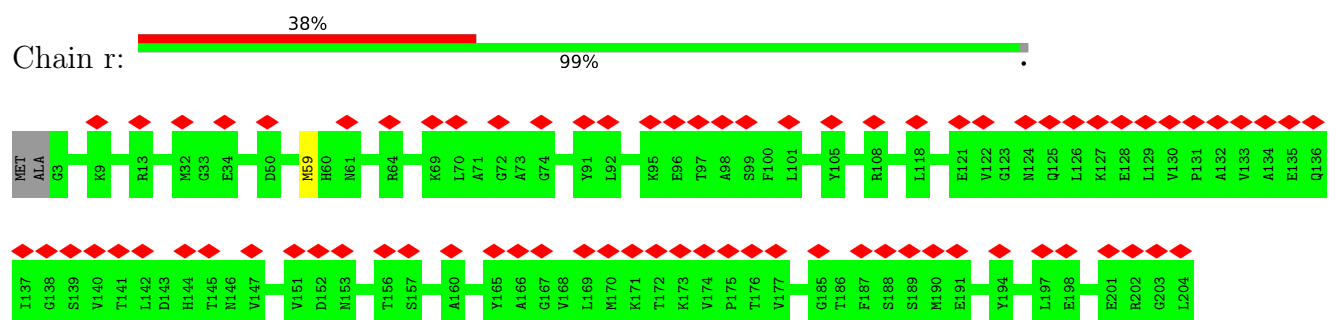
• Molecule 4: Structural protein MCP1



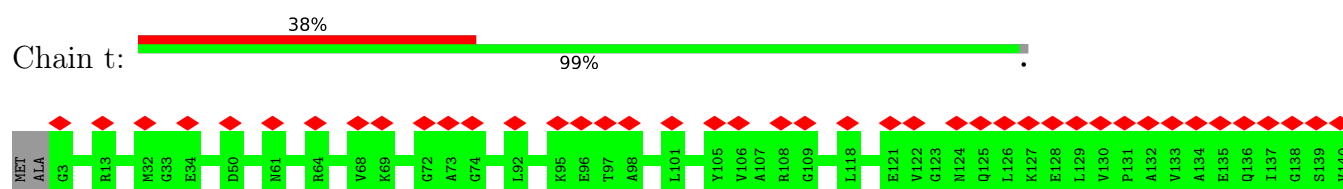
• Molecule 4: Structural protein MCP1



• Molecule 4: Structural protein MCP1



• Molecule 4: Structural protein MCP1





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=38.49°, rise=5.48 Å, axial sym=C1	Depositor
Number of segments used	167500	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0344	Depositor
Map size (Å)	448.0, 448.0, 448.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	1	0.84	0/5175	1.23	22/7985 (0.3%)
2	2	0.85	0/5127	1.25	25/7911 (0.3%)
3	A	0.32	0/1245	0.41	0/1682
3	B	0.32	0/1245	0.42	0/1682
3	C	0.32	0/1245	0.41	0/1682
3	D	0.32	0/1245	0.42	0/1682
3	E	0.32	0/1245	0.43	0/1682
3	F	0.32	0/1245	0.42	0/1682
3	G	0.32	0/1245	0.41	0/1682
3	H	0.32	0/1245	0.42	0/1682
3	I	0.32	0/1245	0.41	0/1682
3	J	0.32	0/1245	0.42	0/1682
3	K	0.32	0/1245	0.41	0/1682
3	L	0.32	0/1245	0.43	0/1682
3	M	0.32	0/1245	0.41	0/1682
3	N	0.32	0/1245	0.42	0/1682
3	P	0.33	0/1245	0.42	0/1682
3	R	0.32	0/1245	0.41	0/1682
3	T	0.32	0/1245	0.41	0/1682
4	a	0.32	0/1580	0.48	0/2151
4	b	0.32	0/1580	0.48	0/2151
4	c	0.33	0/1580	0.47	0/2151
4	d	0.32	0/1580	0.48	0/2151
4	e	0.33	0/1580	0.47	0/2151
4	f	0.32	0/1580	0.47	0/2151
4	g	0.33	0/1580	0.47	0/2151
4	h	0.33	0/1580	0.47	0/2151
4	i	0.33	0/1580	0.48	0/2151
4	j	0.33	0/1580	0.47	0/2151
4	k	0.32	0/1580	0.48	0/2151
4	l	0.32	0/1580	0.47	0/2151
4	m	0.33	0/1580	0.48	0/2151
4	n	0.33	0/1580	0.47	0/2151
4	p	0.33	0/1580	0.48	0/2151

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	r	0.32	0/1580	0.47	0/2151
4	t	0.32	0/1580	0.47	0/2151
All	All	0.46	0/58327	0.68	47/81057 (0.1%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	150	DT	O4'-C1'-N1	7.25	113.08	108.00
2	2	382	DT	O4'-C4'-C3'	-6.93	101.73	104.50
2	2	322	DT	O4'-C4'-C3'	-6.86	101.75	104.50
1	1	150	DT	O4'-C4'-C3'	-6.74	101.81	104.50
2	2	418	DT	O4'-C4'-C3'	-6.53	101.89	104.50
1	1	230	DT	O4'-C4'-C3'	-6.46	101.91	104.50
2	2	370	DT	O4'-C4'-C3'	-6.45	101.92	104.50
2	2	298	DT	O4'-C4'-C3'	-6.38	101.95	104.50
2	2	430	DT	O4'-C4'-C3'	-6.31	101.98	104.50
1	1	168	DT	O4'-C4'-C3'	-6.29	101.98	104.50
2	2	442	DT	O4'-C4'-C3'	-6.15	102.04	104.50
1	1	204	DT	O4'-C4'-C3'	-6.02	102.09	104.50
2	2	466	DT	O4'-C4'-C3'	-5.86	102.16	104.50
2	2	478	DT	O4'-C4'-C3'	-5.83	102.17	104.50
1	1	228	DT	O4'-C4'-C3'	-5.83	102.17	104.50
2	2	462	DT	O4'-C4'-C3'	-5.82	102.17	104.50
1	1	120	DT	O4'-C4'-C3'	-5.81	102.18	104.50
2	2	454	DT	O4'-C4'-C3'	-5.73	102.21	104.50
2	2	294	DT	O4'-C4'-C3'	-5.72	102.21	104.50
1	1	72	DT	O4'-C4'-C3'	-5.70	102.22	104.50
1	1	156	DT	O4'-C4'-C3'	-5.61	102.26	104.50
1	1	84	DT	O4'-C4'-C3'	-5.58	102.27	104.50
1	1	24	DT	O4'-C4'-C3'	-5.57	102.27	104.50
1	1	60	DT	O4'-C4'-C3'	-5.57	102.27	104.50
2	2	334	DT	O4'-C4'-C3'	-5.54	102.28	104.50
2	2	390	DT	O4'-C4'-C3'	-5.53	102.29	104.50
2	2	346	DT	O4'-C4'-C3'	-5.42	102.33	104.50
1	1	39	DA	O4'-C4'-C3'	-5.39	102.34	104.50
1	1	216	DT	O4'-C4'-C3'	-5.37	102.35	104.50
2	2	310	DT	O4'-C4'-C3'	-5.35	102.36	104.50
1	1	159	DA	O4'-C4'-C3'	-5.34	102.36	104.50
1	1	218	DT	O4'-C4'-C3'	-5.32	102.37	104.50
1	1	27	DA	O4'-C4'-C3'	-5.29	102.38	104.50
2	2	402	DT	OP2-P-O3'	5.27	116.80	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	342	DT	O4'-C4'-C3'	-5.26	102.40	104.50
1	1	171	DA	O4'-C4'-C3'	-5.25	102.40	104.50
1	1	51	DA	O4'-C4'-C3'	-5.15	102.44	104.50
1	1	132	DT	O4'-C4'-C3'	-5.14	102.44	104.50
2	2	394	DT	O4'-C4'-C3'	-5.12	102.45	104.50
2	2	450	DT	N3-C4-O4	5.12	122.97	119.90
2	2	452	DT	O4'-C4'-C3'	-5.11	102.45	104.50
2	2	282	DT	N3-C4-O4	5.10	122.96	119.90
1	1	192	DT	O4'-C4'-C3'	-5.08	102.47	104.50
2	2	414	DT	N3-C4-O4	5.07	122.94	119.90
2	2	488	DT	O4'-C4'-C3'	-5.03	102.49	104.50
2	2	366	DT	N3-C4-O4	5.01	122.91	119.90
1	1	114	DT	N3-C4-O4	5.01	122.90	119.90

There are no chirality outliers.

There are no planarity outliers.

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	
3	A	150/167 (90%)	142 (95%)	8 (5%)	0	100	100
3	B	150/167 (90%)	144 (96%)	6 (4%)	0	100	100
3	C	150/167 (90%)	142 (95%)	8 (5%)	0	100	100
3	D	150/167 (90%)	144 (96%)	6 (4%)	0	100	100
3	E	150/167 (90%)	143 (95%)	7 (5%)	0	100	100
3	F	150/167 (90%)	140 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	150/167 (90%)	142 (95%)	8 (5%)	0	100	100
3	H	150/167 (90%)	142 (95%)	8 (5%)	0	100	100
3	I	150/167 (90%)	142 (95%)	8 (5%)	0	100	100
3	J	150/167 (90%)	143 (95%)	7 (5%)	0	100	100
3	K	150/167 (90%)	144 (96%)	6 (4%)	0	100	100
3	L	150/167 (90%)	144 (96%)	6 (4%)	0	100	100
3	M	150/167 (90%)	144 (96%)	6 (4%)	0	100	100
3	N	150/167 (90%)	142 (95%)	8 (5%)	0	100	100
3	P	150/167 (90%)	145 (97%)	5 (3%)	0	100	100
3	R	150/167 (90%)	141 (94%)	9 (6%)	0	100	100
3	T	150/167 (90%)	143 (95%)	7 (5%)	0	100	100
4	a	200/204 (98%)	178 (89%)	22 (11%)	0	100	100
4	b	200/204 (98%)	178 (89%)	22 (11%)	0	100	100
4	c	200/204 (98%)	177 (88%)	23 (12%)	0	100	100
4	d	200/204 (98%)	182 (91%)	18 (9%)	0	100	100
4	e	200/204 (98%)	177 (88%)	23 (12%)	0	100	100
4	f	200/204 (98%)	180 (90%)	20 (10%)	0	100	100
4	g	200/204 (98%)	178 (89%)	22 (11%)	0	100	100
4	h	200/204 (98%)	179 (90%)	21 (10%)	0	100	100
4	i	200/204 (98%)	178 (89%)	22 (11%)	0	100	100
4	j	200/204 (98%)	182 (91%)	18 (9%)	0	100	100
4	k	200/204 (98%)	177 (88%)	23 (12%)	0	100	100
4	l	200/204 (98%)	180 (90%)	20 (10%)	0	100	100
4	m	200/204 (98%)	177 (88%)	23 (12%)	0	100	100
4	n	200/204 (98%)	179 (90%)	21 (10%)	0	100	100
4	p	200/204 (98%)	178 (89%)	22 (11%)	0	100	100
4	r	200/204 (98%)	177 (88%)	23 (12%)	0	100	100
4	t	200/204 (98%)	182 (91%)	18 (9%)	0	100	100
All	All	5950/6307 (94%)	5466 (92%)	484 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	128/141 (91%)	128 (100%)	0	100	100
3	B	128/141 (91%)	128 (100%)	0	100	100
3	C	128/141 (91%)	128 (100%)	0	100	100
3	D	128/141 (91%)	128 (100%)	0	100	100
3	E	128/141 (91%)	128 (100%)	0	100	100
3	F	128/141 (91%)	128 (100%)	0	100	100
3	G	128/141 (91%)	128 (100%)	0	100	100
3	H	128/141 (91%)	127 (99%)	1 (1%)	81	89
3	I	128/141 (91%)	128 (100%)	0	100	100
3	J	128/141 (91%)	127 (99%)	1 (1%)	81	89
3	K	128/141 (91%)	128 (100%)	0	100	100
3	L	128/141 (91%)	128 (100%)	0	100	100
3	M	128/141 (91%)	128 (100%)	0	100	100
3	N	128/141 (91%)	127 (99%)	1 (1%)	81	89
3	P	128/141 (91%)	128 (100%)	0	100	100
3	R	128/141 (91%)	128 (100%)	0	100	100
3	T	128/141 (91%)	128 (100%)	0	100	100
4	a	166/172 (96%)	166 (100%)	0	100	100
4	b	166/172 (96%)	165 (99%)	1 (1%)	86	92
4	c	166/172 (96%)	166 (100%)	0	100	100
4	d	166/172 (96%)	166 (100%)	0	100	100
4	e	166/172 (96%)	166 (100%)	0	100	100
4	f	166/172 (96%)	166 (100%)	0	100	100
4	g	166/172 (96%)	166 (100%)	0	100	100
4	h	166/172 (96%)	166 (100%)	0	100	100
4	i	166/172 (96%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	j	166/172 (96%)	166 (100%)	0	100	100
4	k	166/172 (96%)	166 (100%)	0	100	100
4	l	166/172 (96%)	166 (100%)	0	100	100
4	m	166/172 (96%)	166 (100%)	0	100	100
4	n	166/172 (96%)	166 (100%)	0	100	100
4	p	166/172 (96%)	166 (100%)	0	100	100
4	r	166/172 (96%)	165 (99%)	1 (1%)	86	92
4	t	166/172 (96%)	166 (100%)	0	100	100
All	All	4998/5321 (94%)	4993 (100%)	5 (0%)	93	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	115	PHE
3	J	115	PHE
3	N	115	PHE
4	b	186	THR
4	r	59	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	112	HIS
3	B	112	HIS
3	C	30	HIS
3	D	112	HIS
3	E	30	HIS
3	E	112	HIS
3	F	112	HIS
3	G	30	HIS
3	G	112	HIS
3	H	30	HIS
3	H	113	HIS
3	I	30	HIS
3	I	112	HIS
3	J	24	ASN
3	J	52	GLN
3	J	112	HIS

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Mol	Chain	Res	Type
3	K	30	HIS
3	K	112	HIS
3	L	112	HIS
3	M	30	HIS
3	M	112	HIS
3	N	30	HIS
3	N	112	HIS
3	P	112	HIS
3	R	30	HIS
3	R	112	HIS
3	T	52	GLN
3	T	112	HIS
4	a	30	ASN
4	a	180	HIS
4	b	30	ASN
4	b	57	ASN
4	b	180	HIS
4	c	30	ASN
4	c	57	ASN
4	d	30	ASN
4	d	38	GLN
4	e	30	ASN
4	f	57	ASN
4	g	30	ASN
4	g	38	GLN
4	g	153	ASN
4	h	30	ASN
4	h	57	ASN
4	h	124	ASN
4	h	180	HIS
4	i	57	ASN
4	i	180	HIS
4	j	38	GLN
4	j	57	ASN
4	j	124	ASN
4	j	153	ASN
4	k	30	ASN
4	k	136	GLN
4	l	30	ASN
4	m	30	ASN
4	n	30	ASN
4	n	57	ASN

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Mol	Chain	Res	Type
4	n	136	GLN
4	n	153	ASN
4	p	153	ASN
4	r	30	ASN
4	r	57	ASN
4	r	180	HIS
4	t	30	ASN
4	t	49	ASN
4	t	57	ASN
4	t	180	HIS

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.

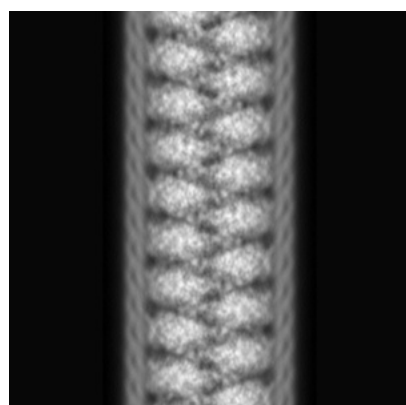
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21868. These allow visual inspection of the internal detail of the map and identification of artifacts.

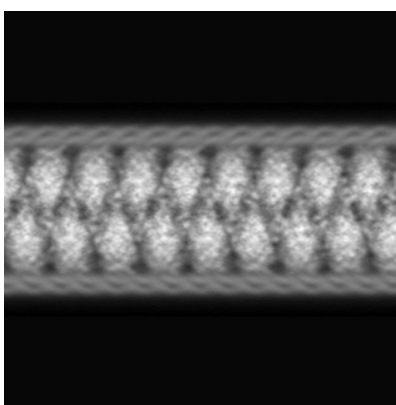
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

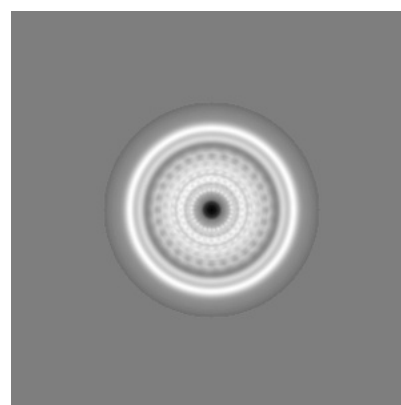
6.1.1 Primary map



X



Y

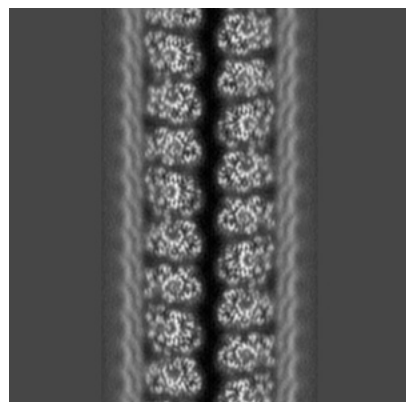


Z

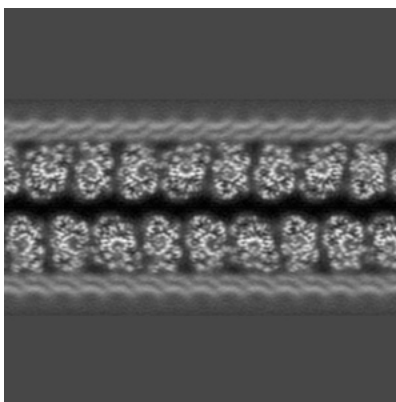
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

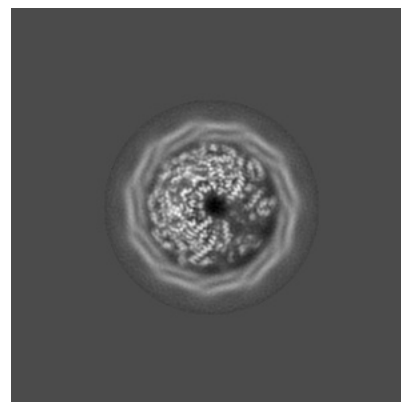
6.2.1 Primary map



X Index: 160



Y Index: 160

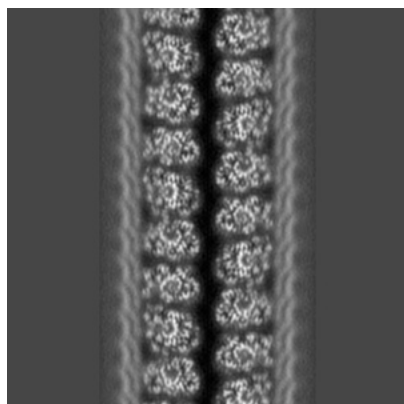


Z Index: 160

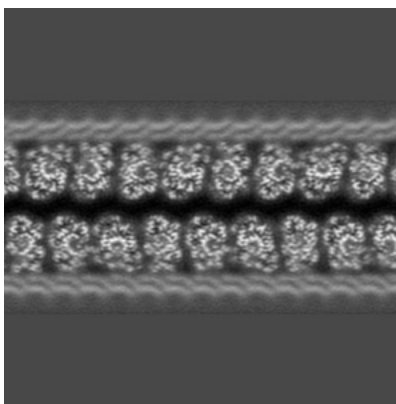
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

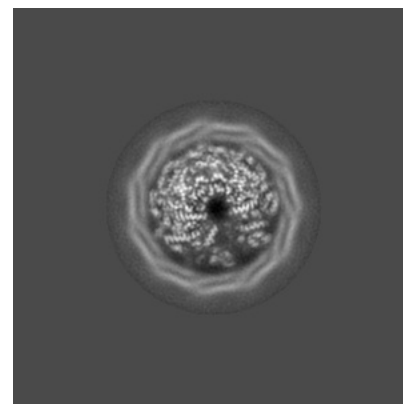
6.3.1 Primary map



X Index: 160



Y Index: 159

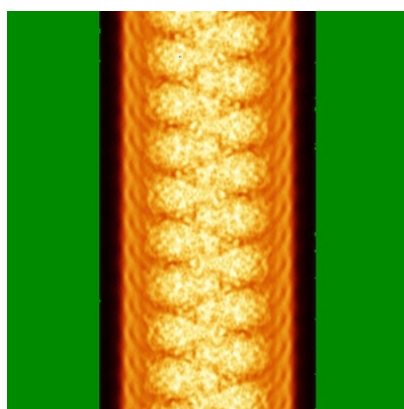


Z Index: 46

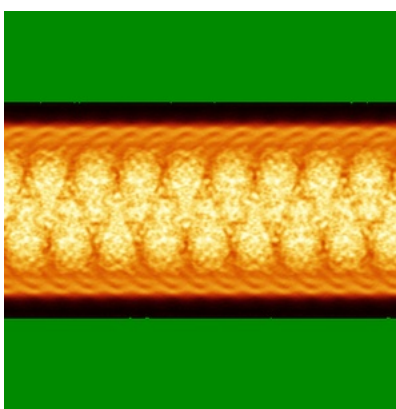
The images above show the largest variance slices of the map in three orthogonal directions.

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

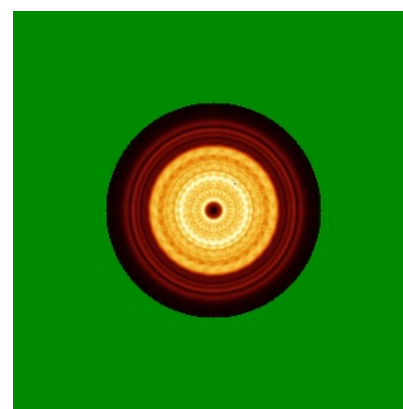
6.4.1 Primary map



X



Y

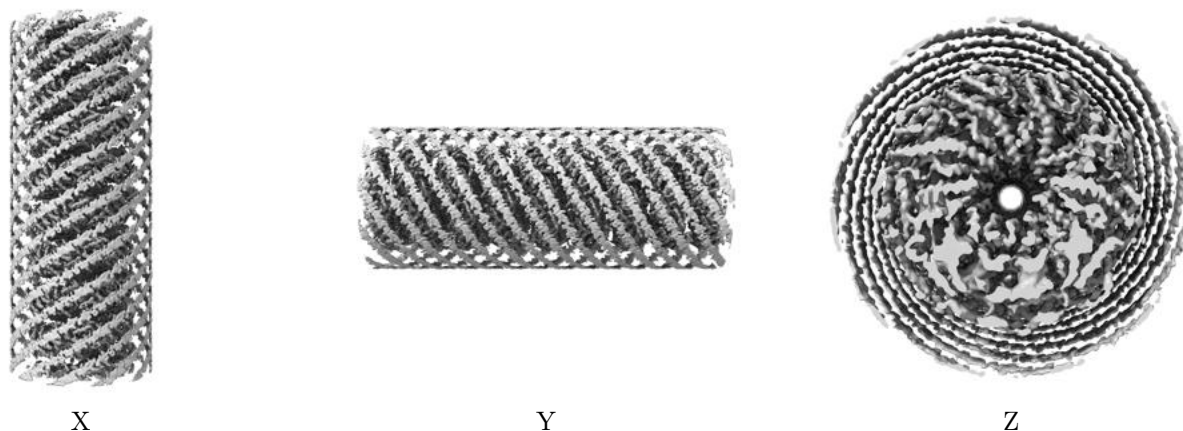


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0344. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

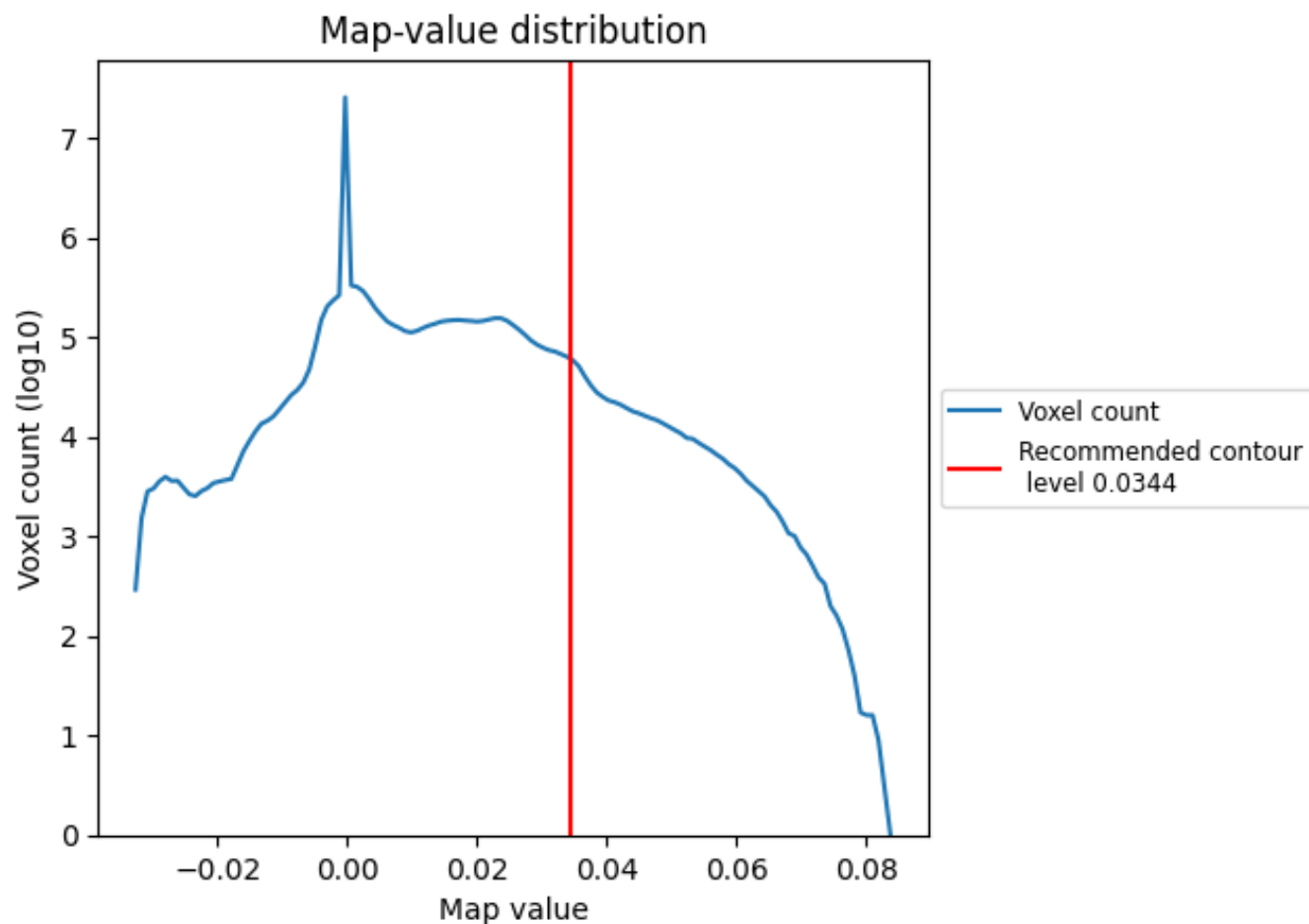
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

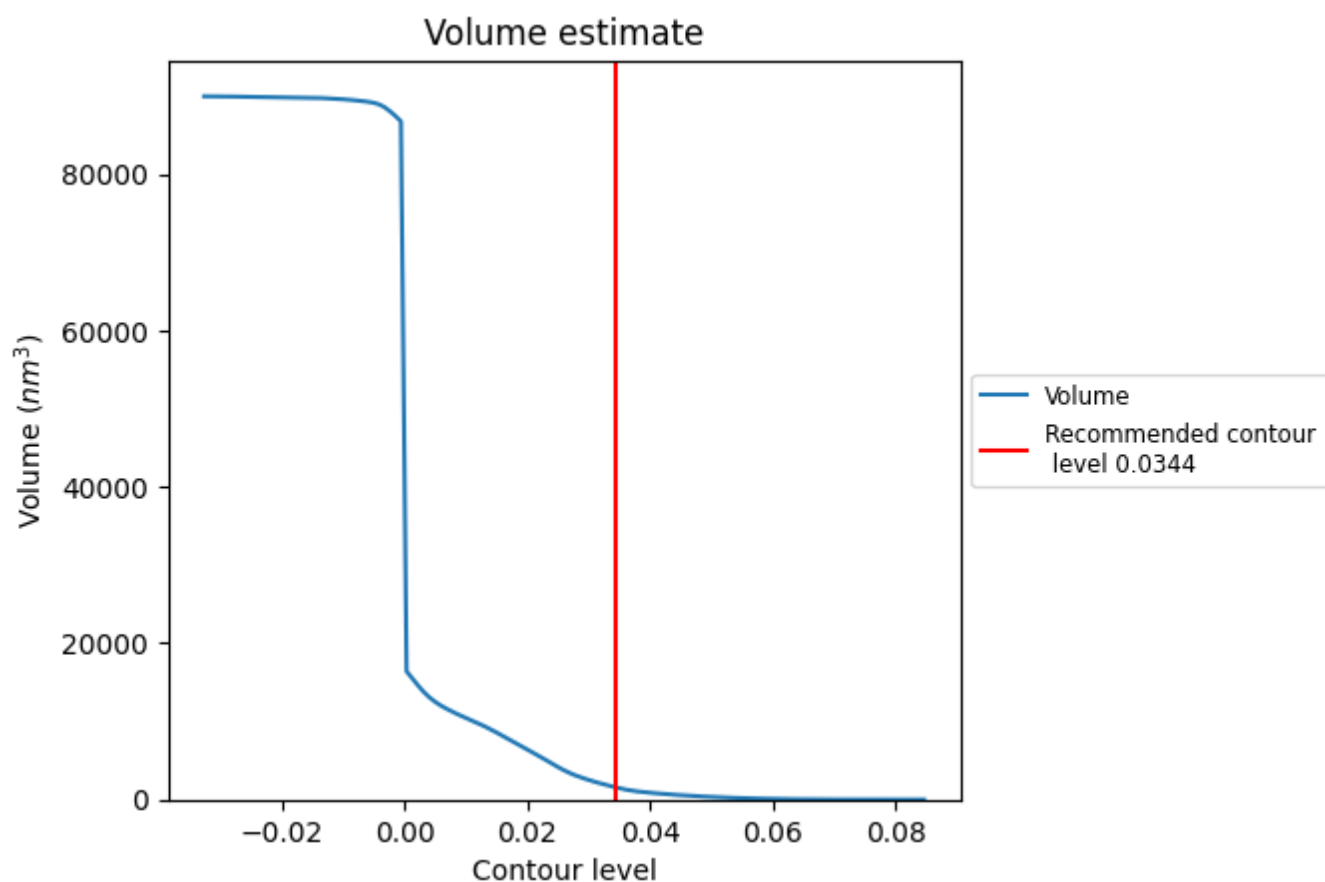
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

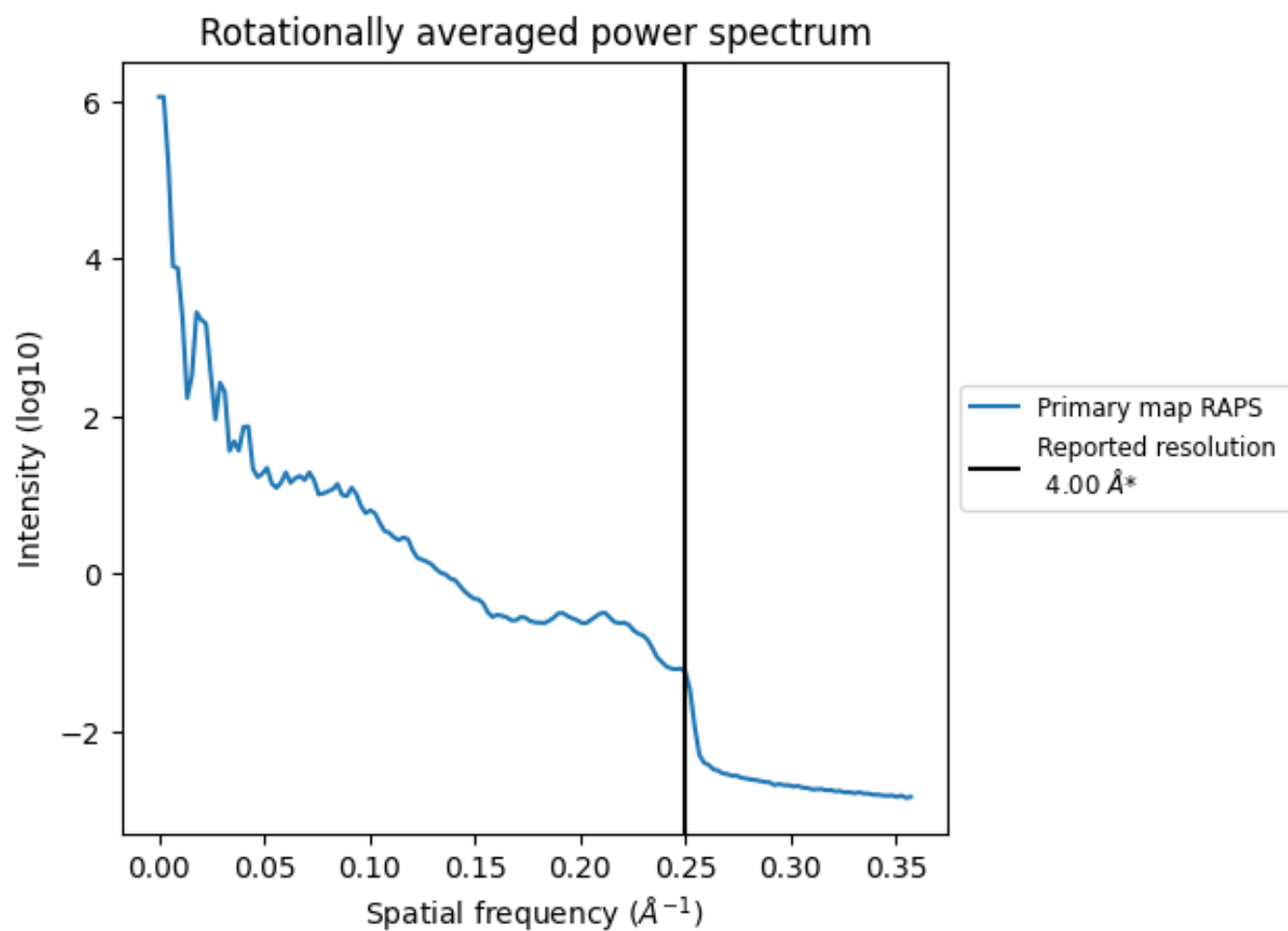
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1570 nm³; this corresponds to an approximate mass of 1418 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 0.250 Å⁻¹

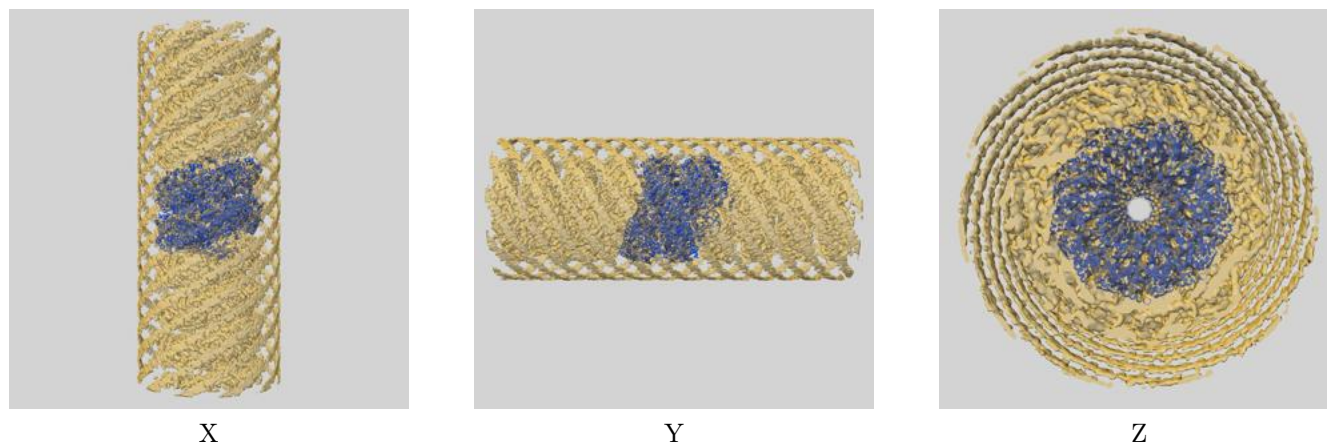
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

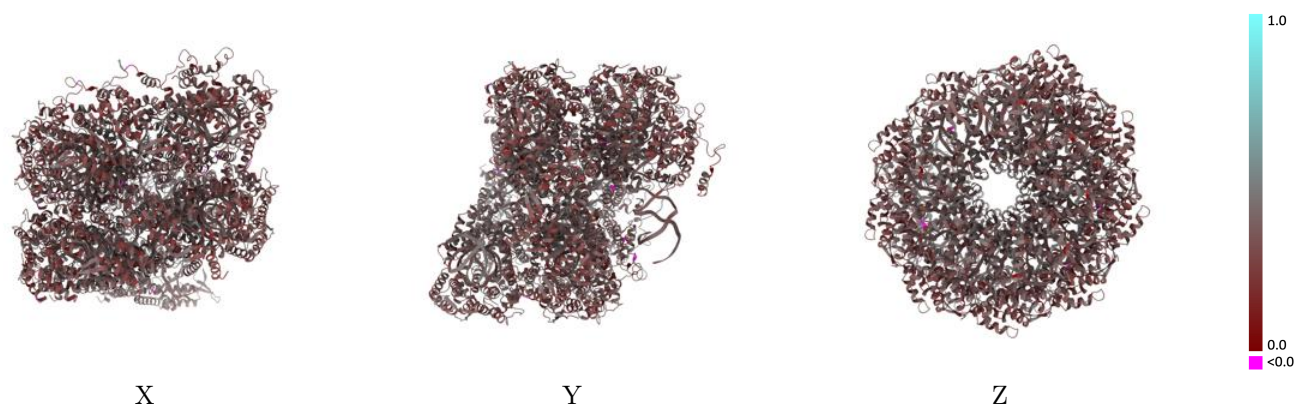
This section contains information regarding the fit between EMDB map EMD-21868 and PDB model 6WQ2. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



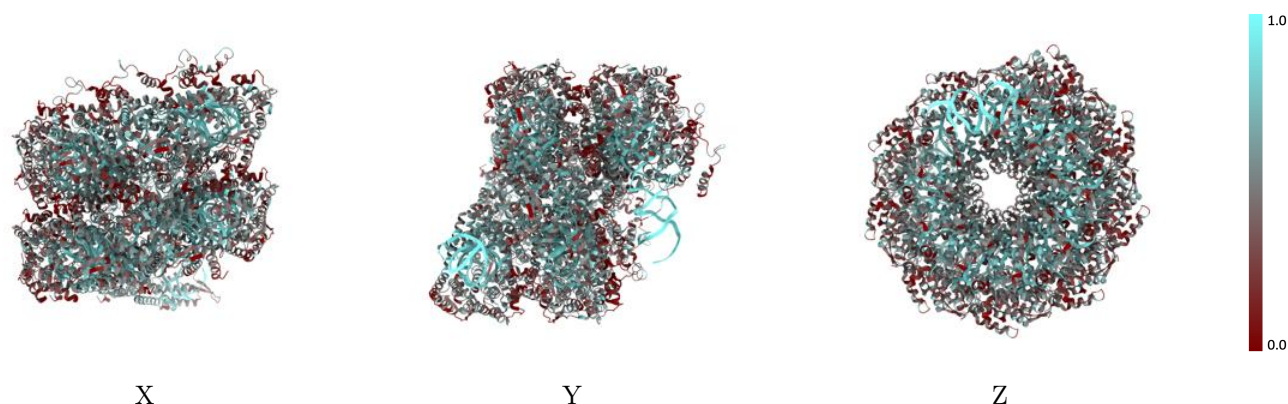
The images above show the 3D surface view of the map at the recommended contour level 0.0344 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



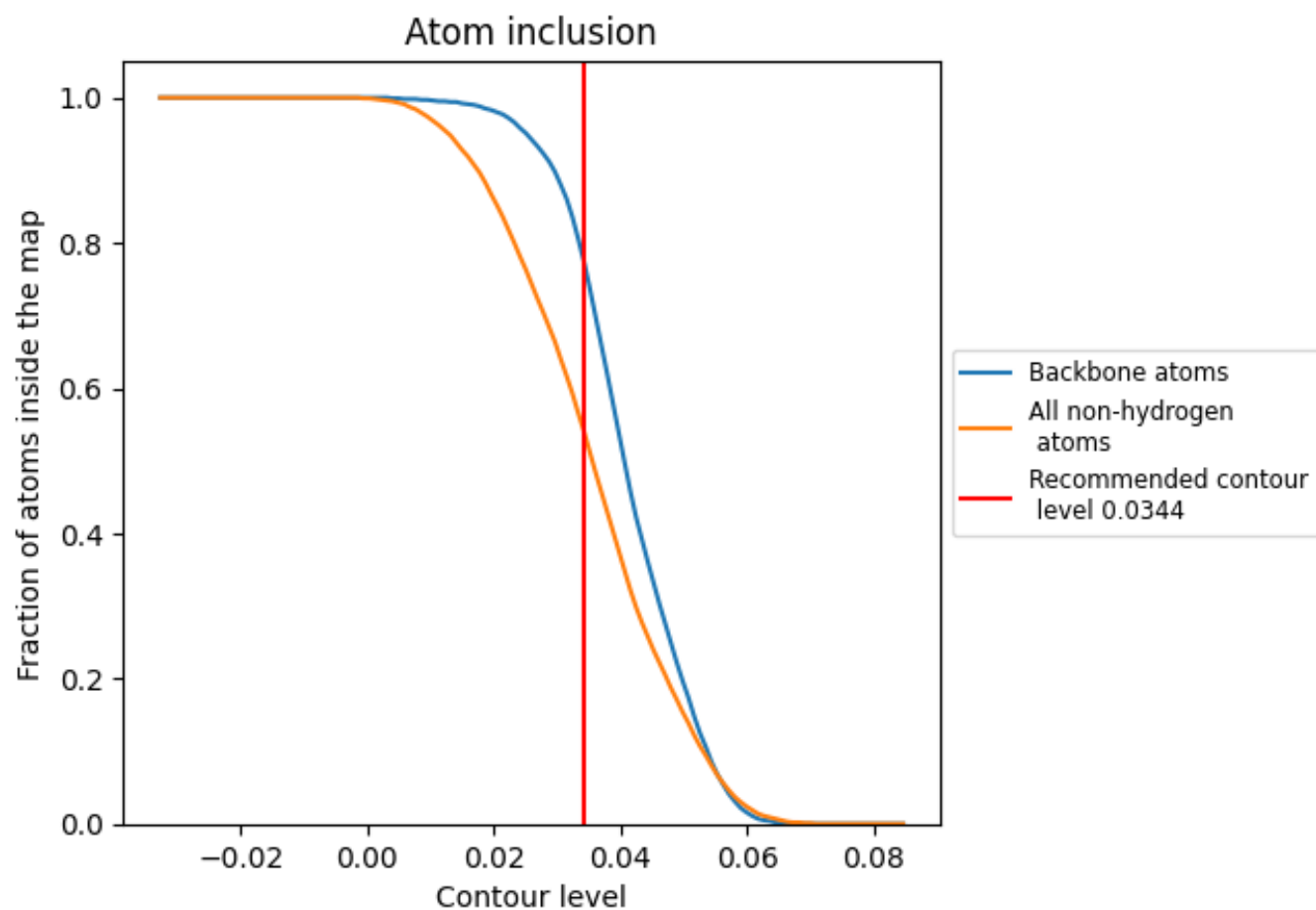
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0344).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 54% 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 (0.0344) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5370	 0.3420
1	 0.9010	 0.3610
2	 0.9190	 0.3570
A	 0.4820	 0.3410
B	 0.4790	 0.3390
C	 0.4860	 0.3410
D	 0.4820	 0.3410
E	 0.4840	 0.3420
F	 0.4910	 0.3450
G	 0.4800	 0.3420
H	 0.4900	 0.3460
I	 0.4820	 0.3430
J	 0.4900	 0.3400
K	 0.4800	 0.3400
L	 0.4810	 0.3380
M	 0.4780	 0.3430
N	 0.4830	 0.3380
P	 0.4740	 0.3410
R	 0.4790	 0.3390
T	 0.4740	 0.3390
a	 0.4480	 0.3330
b	 0.4500	 0.3350
c	 0.4560	 0.3380
d	 0.4460	 0.3370
e	 0.4440	 0.3330
f	 0.4430	 0.3350
g	 0.4480	 0.3380
h	 0.4430	 0.3380
i	 0.4510	 0.3370
j	 0.4450	 0.3380
k	 0.4420	 0.3380
l	 0.4550	 0.3390
m	 0.4420	 0.3390
n	 0.4450	 0.3380
p	 0.4500	 0.3380



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Chain	Atom inclusion	Q-score
r	 0.4510	 0.3350
t	 0.4450	 0.3360