



Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 08:18 am BST

PDB ID : 7OKO
EMDB ID : EMD-12963
Title : Structure of the outer-membrane core complex (outer ring) from a conjugative type IV secretion system
Authors : Amin, H.; Ilangoan, A.; Costa, T.R.D.
Deposited on : 2021-05-18
Resolution : 3.40 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:

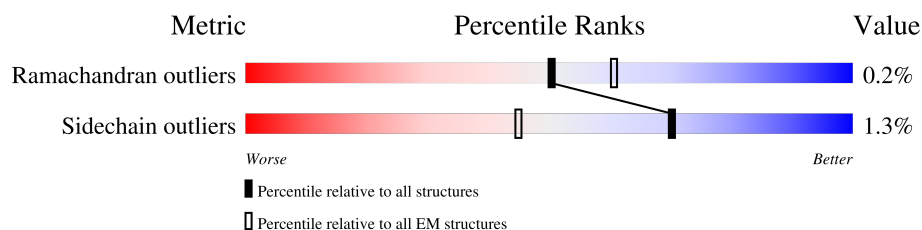
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.








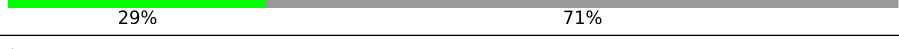

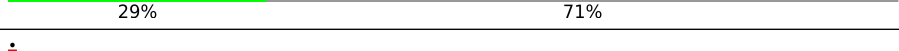
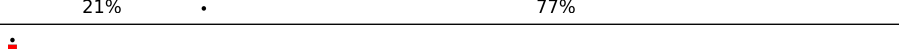
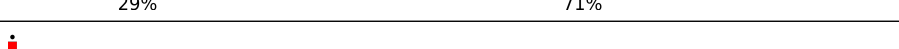






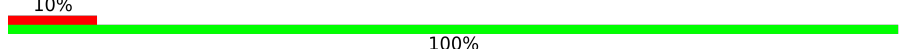
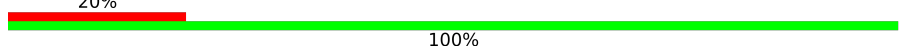
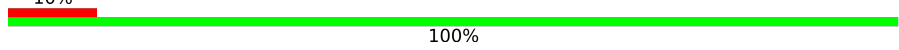
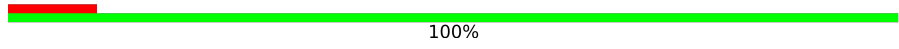
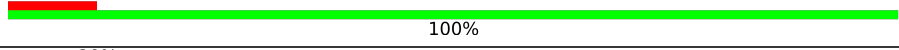
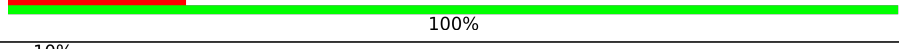
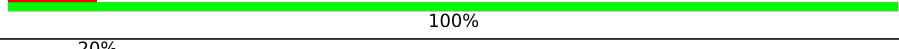
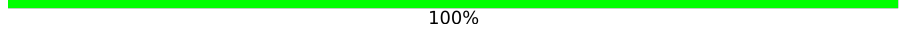

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	0	204	
1	1	204	
1	5	204	
1	6	204	
1	AA	204	
1	AB	204	
1	C	204	
1	D	204	
1	H	204	

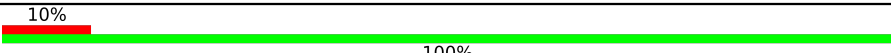

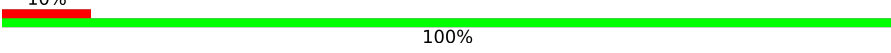
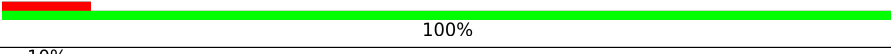
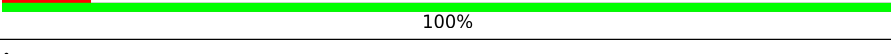
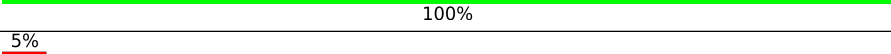
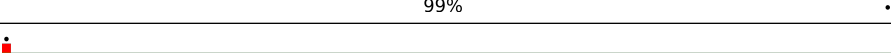
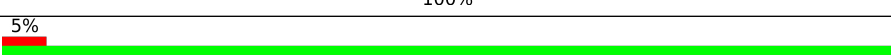
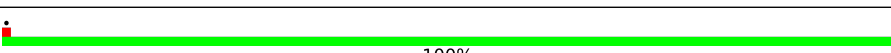
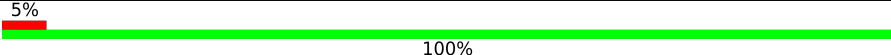
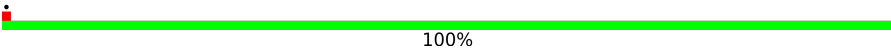
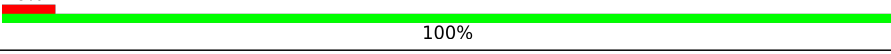
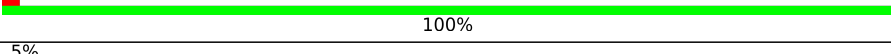
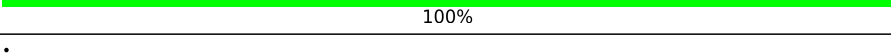
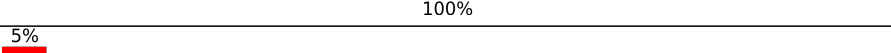
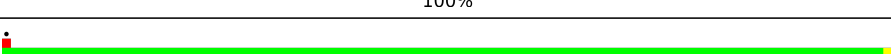
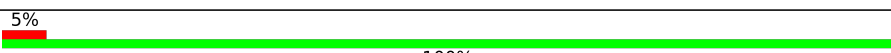
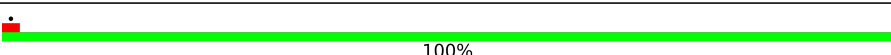
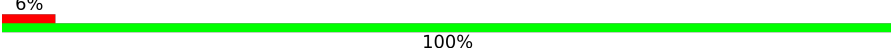
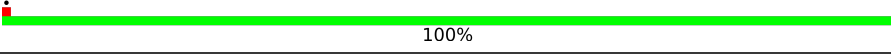
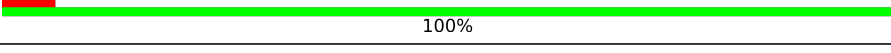
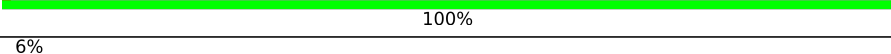
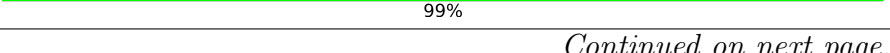


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Mol	Chain	Length	Quality of chain
1	I	204	
1	M	204	
1	N	204	
1	R	204	
1	S	204	
1	W	204	
1	X	204	
1	b	204	
1	c	204	
1	g	204	
1	h	204	
1	l	204	
1	m	204	
1	q	204	
1	r	204	
1	v	204	
1	w	204	
2	2	10	
2	7	10	
2	AC	10	
2	E	10	
2	J	10	
2	O	10	
2	T	10	
2	Y	10	

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Mol	Chain	Length	Quality of chain
2	d	10	
2	i	10	
2	n	10	
2	s	10	
2	x	10	
3	3	216	
3	4	216	
3	8	216	
3	9	216	
3	A	216	
3	B	216	
3	F	216	
3	G	216	
3	K	216	
3	L	216	
3	P	216	
3	Q	216	
3	U	216	
3	V	216	
3	Z	216	
3	a	216	
3	e	216	
3	f	216	
3	j	216	
3	k	216	

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Mol	Chain	Length	Quality of chain
3	o	216	 100%
3	p	216	 100%
3	t	216	 100%
3	u	216	 100%
3	y	216	 100%
3	z	216	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 54483 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 Type IV conjugative transfer system lipoprotein TraV.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AA	46	Total	C	N	O	0	0
			370	238	69	63		
1	AB	60	Total	C	N	O	0	0
			467	294	87	86		
1	0	60	Total	C	N	O	0	0
			467	294	87	86		
1	1	46	Total	C	N	O	0	0
			370	238	69	63		
1	5	60	Total	C	N	O	0	0
			467	294	87	86		
1	6	46	Total	C	N	O	0	0
			370	238	69	63		
1	C	60	Total	C	N	O	0	0
			467	294	87	86		
1	D	46	Total	C	N	O	0	0
			370	238	69	63		
1	H	60	Total	C	N	O	0	0
			467	294	87	86		
1	I	46	Total	C	N	O	0	0
			370	238	69	63		
1	M	60	Total	C	N	O	0	0
			467	294	87	86		
1	N	46	Total	C	N	O	0	0
			370	238	69	63		
1	R	60	Total	C	N	O	0	0
			467	294	87	86		
1	S	46	Total	C	N	O	0	0
			370	238	69	63		
1	W	60	Total	C	N	O	0	0
			467	294	87	86		
1	X	46	Total	C	N	O	0	0
			370	238	69	63		
1	b	60	Total	C	N	O	0	0
			467	294	87	86		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	c	46	Total	C	N	O	0	0
			370	238	69	63		
1	g	60	Total	C	N	O	0	0
			467	294	87	86		
1	h	46	Total	C	N	O	0	0
			370	238	69	63		
1	l	60	Total	C	N	O	0	0
			467	294	87	86		
1	m	46	Total	C	N	O	0	0
			370	238	69	63		
1	q	60	Total	C	N	O	0	0
			467	294	87	86		
1	r	46	Total	C	N	O	0	0
			370	238	69	63		
1	v	60	Total	C	N	O	0	0
			467	294	87	86		
1	w	46	Total	C	N	O	0	0
			370	238	69	63		

- Molecule 2 is a protein called TraB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	2	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	7	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	E	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	J	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	O	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	T	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	Y	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	d	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	i	10	Total	C	N	O	S	0	0
			76	46	11	17	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	n	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	s	10	Total	C	N	O	S	0	0
			76	46	11	17	2		
2	x	10	Total	C	N	O	S	0	0
			76	46	11	17	2		

- Molecule 3 is a protein called Type-F conjugative transfer system secretin TraK.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	4	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	8	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	9	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	A	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	B	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	F	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	G	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	K	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	L	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	P	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	Q	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	U	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	V	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	Z	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		
3	a	216	Total	C	N	O	S	0	0
			1639	1035	292	306	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	f	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	j	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	k	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	o	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	p	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	t	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	u	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	y	216	Total 1639	C 1035	N 292	O 306	S 6	0	0
3	z	216	Total 1639	C 1035	N 292	O 306	S 6	0	0



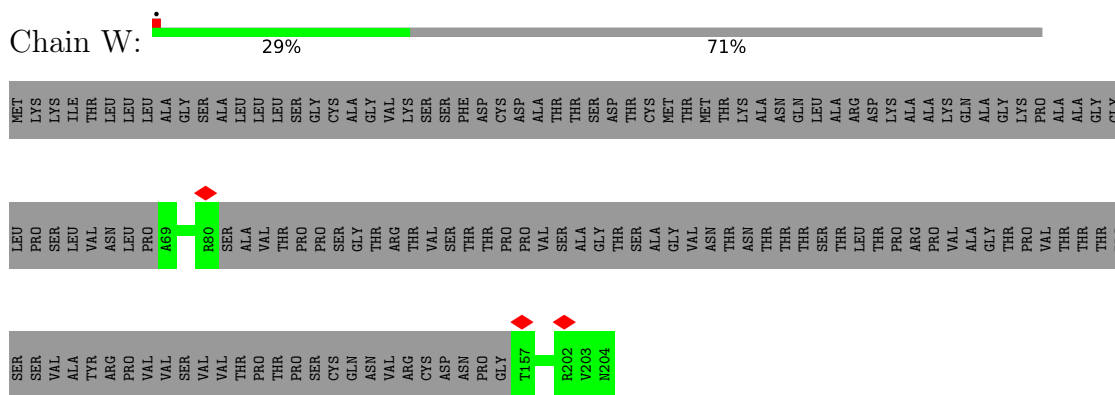


- Molecule 1: Type IV conjugative transfer system lipoprotein TraV

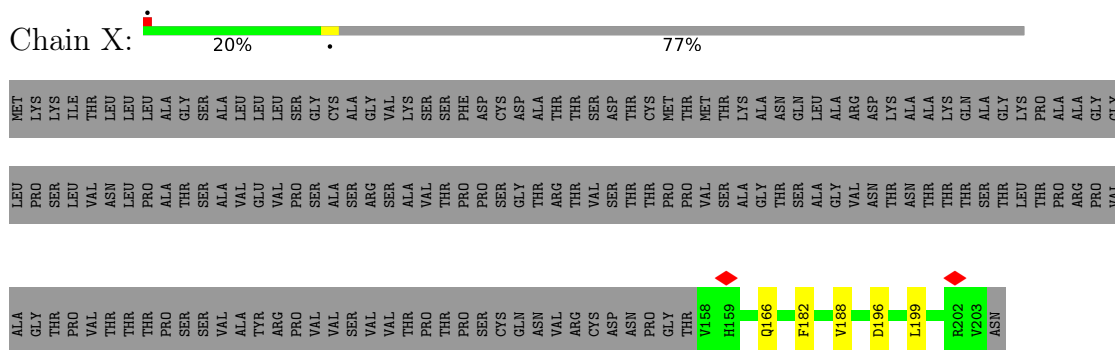
- Molecule 1: Type IV conjugative transfer system lipoprotein TraV

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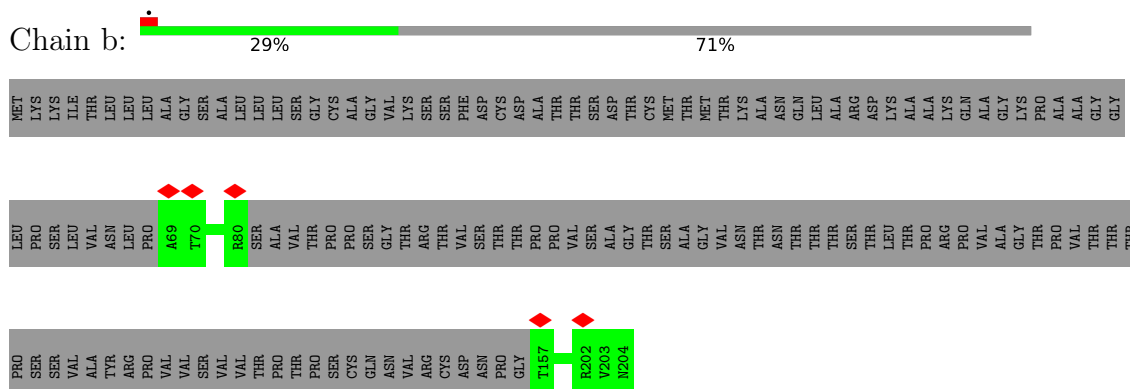
- Molecule 1: Type IV conjugative transfer system lipoprotein TraV



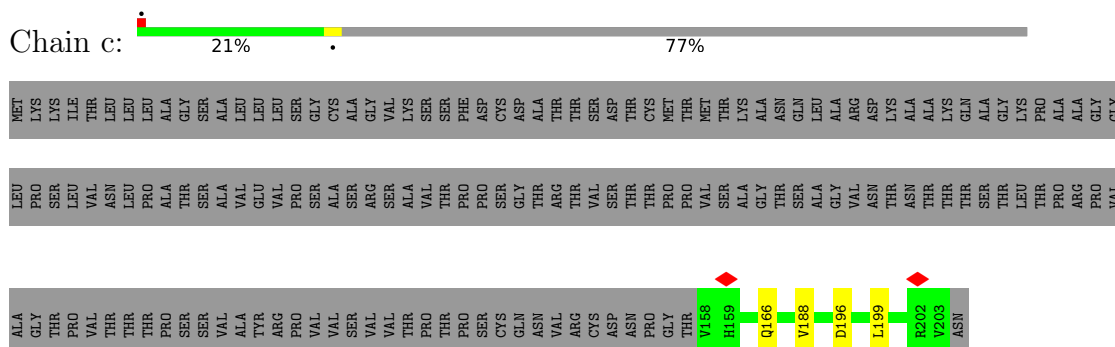
- Molecule 1: Type IV conjugative transfer system lipoprotein TraV



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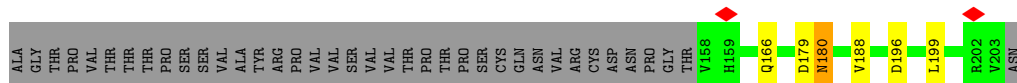


- Molecule 1: Type IV conjugative transfer system lipoprotein TraV



- [illegible]





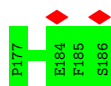
Chain AC:  10% 100%



Chain 2:  10% 100%



Chain 7:  20% 100%



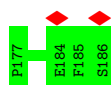
Chain E:  10% 100%



Chain J: 



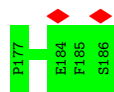
Chain O:  20% 100%



• Molecule 2: TraB



• Molecule 2: TraB



• Molecule 2: TraB



• Molecule 2: TraB



• Molecule 2: TraB



• Molecule 2: TraB



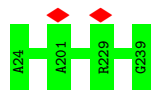
• Molecule 2: TraB





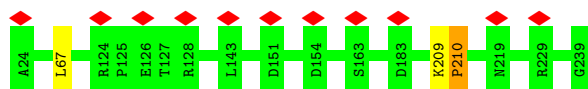
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain 3: 100%



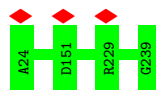
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain 4: 5% 99%



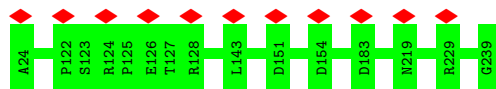
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain 8: 100%



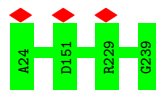
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain 9: 5% 100%



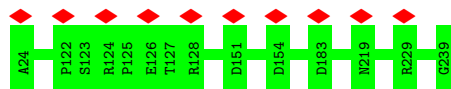
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain A: 100%



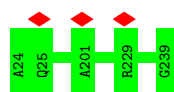
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain B: 5% 100%



- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain F:  100%



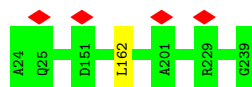
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain G:  6%  100%



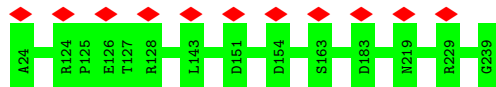
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain K:  100%



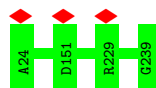
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain L:  5%  100%



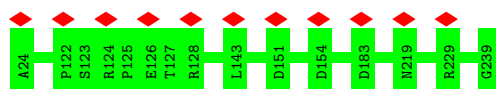
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain P:  100%



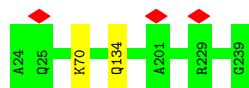
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain Q:  5%  100%



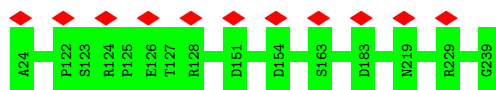
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain U:  99%



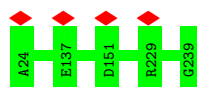
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain V:  5% 100%



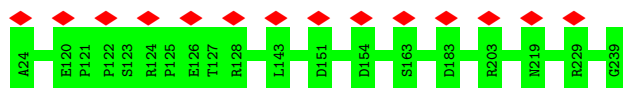
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain Z:  1% 100%



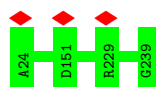
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain a:  6% 100%



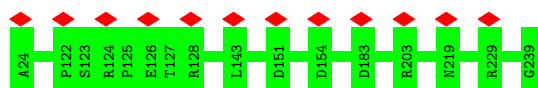
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain e:  1% 100%



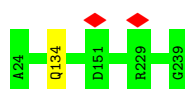
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain f:  6% 100%



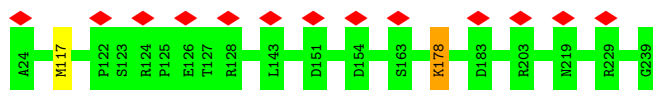
- Molecule 3: Type-F conjugative transfer system secretin TraK

Chain j:  1% 100%

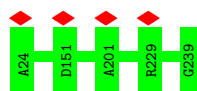


- Molecule 3: Type-F conjugative transfer system secretin TraK

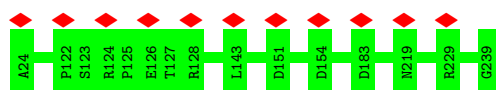
Chain k:  6% 99%



- Molecule 3: Type-F conjugative transfer system secretin TraK



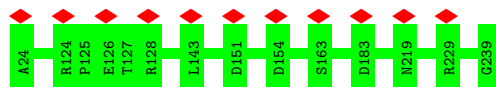
- Molecule 3: Type-F conjugative transfer system secretin TraK



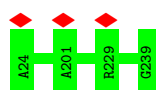
- Molecule 3: Type-F conjugative transfer system secretin TraK



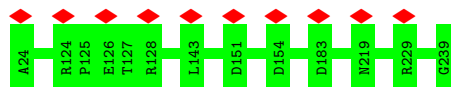
- Molecule 3: Type-F conjugative transfer system secretin TraK



- Molecule 3: Type-F conjugative transfer system secretin TraK



- Molecule 3: Type-F conjugative transfer system secretin TraK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.688	Depositor
Minimum map value	-0.623	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.31	0/481	0.44	0/661
1	1	0.42	0/384	0.58	0/530
1	5	0.31	0/481	0.44	0/661
1	6	0.42	0/384	0.59	0/530
1	AA	0.42	0/384	0.62	0/530
1	AB	0.31	0/481	0.44	0/661
1	C	0.31	0/481	0.44	0/661
1	D	0.42	0/384	0.60	0/530
1	H	0.30	0/481	0.44	0/661
1	I	0.37	0/384	0.63	1/530 (0.2%)
1	M	0.31	0/481	0.44	0/661
1	N	0.42	0/384	0.61	0/530
1	R	0.31	0/481	0.44	0/661
1	S	0.41	0/384	0.60	0/530
1	W	0.30	0/481	0.44	0/661
1	X	0.38	0/384	0.68	1/530 (0.2%)
1	b	0.31	0/481	0.44	0/661
1	c	0.38	0/384	0.60	0/530
1	g	0.31	0/481	0.44	0/661
1	h	0.42	0/384	0.60	0/530
1	l	0.31	0/481	0.44	0/661
1	m	0.42	0/384	0.61	0/530
1	q	0.31	0/481	0.44	0/661
1	r	0.42	0/384	0.61	0/530
1	v	0.31	0/481	0.44	0/661
1	w	0.41	0/384	0.60	0/530
2	2	0.33	0/77	0.48	0/100
2	7	0.33	0/77	0.48	0/100
2	AC	0.33	0/77	0.48	0/100
2	E	0.33	0/77	0.48	0/100
2	J	0.33	0/77	0.48	0/100
2	O	0.33	0/77	0.48	0/100
2	T	0.33	0/77	0.48	0/100
2	Y	0.33	0/77	0.48	0/100

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	d	0.33	0/77	0.48	0/100
2	i	0.33	0/77	0.48	0/100
2	n	0.33	0/77	0.48	0/100
2	s	0.33	0/77	0.48	0/100
2	x	0.33	0/77	0.48	0/100
3	3	0.33	0/1673	0.50	0/2273
3	4	0.34	0/1673	0.57	1/2273 (0.0%)
3	8	0.32	0/1673	0.51	0/2273
3	9	0.31	0/1673	0.53	0/2273
3	A	0.33	0/1673	0.51	0/2273
3	B	0.32	0/1673	0.52	0/2273
3	F	0.32	0/1673	0.50	0/2273
3	G	0.32	0/1673	0.54	0/2273
3	K	0.33	0/1673	0.53	1/2273 (0.0%)
3	L	0.32	0/1673	0.53	0/2273
3	P	0.33	0/1673	0.50	0/2273
3	Q	0.33	0/1673	0.55	0/2273
3	U	0.33	0/1673	0.51	0/2273
3	V	0.34	0/1673	0.55	0/2273
3	Z	0.33	0/1673	0.53	0/2273
3	a	0.33	0/1673	0.54	0/2273
3	e	0.33	0/1673	0.51	0/2273
3	f	0.32	0/1673	0.55	0/2273
3	j	0.33	0/1673	0.52	0/2273
3	k	0.34	0/1673	0.56	1/2273 (0.0%)
3	o	0.33	0/1673	0.51	0/2273
3	p	0.31	0/1673	0.53	0/2273
3	t	0.33	0/1673	0.51	0/2273
3	u	0.32	0/1673	0.53	0/2273
3	y	0.33	0/1673	0.51	0/2273
3	z	0.31	0/1673	0.54	0/2273
All	All	0.33	0/55744	0.53	5/75881 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	182	PHE	CB-CA-C	-8.15	94.10	110.40
1	I	182	PHE	CB-CA-C	-5.91	98.58	110.40
3	4	67	LEU	CA-CB-CG	5.61	128.19	115.30
3	k	178	LYS	CD-CE-NZ	-5.54	98.96	111.70
3	K	162	LEU	CA-CB-CG	5.10	127.03	115.30

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	
1	0	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	1	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
1	5	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	6	44/204 (22%)	42 (96%)	1 (2%)	1 (2%)	6	28
1	AA	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
1	AB	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	C	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	D	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
1	H	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	I	44/204 (22%)	42 (96%)	2 (4%)	0	100	100
1	M	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	N	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
1	R	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	S	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
1	W	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	X	44/204 (22%)	42 (96%)	2 (4%)	0	100	100
1	b	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	c	44/204 (22%)	42 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	h	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
1	l	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	m	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
1	q	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	r	44/204 (22%)	42 (96%)	1 (2%)	1 (2%)	6	28
1	v	56/204 (28%)	53 (95%)	3 (5%)	0	100	100
1	w	44/204 (22%)	41 (93%)	2 (4%)	1 (2%)	6	28
2	2	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	7	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	AC	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	E	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	J	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	O	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	T	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	Y	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	d	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	i	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	n	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	s	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	x	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	3	214/216 (99%)	181 (85%)	33 (15%)	0	100	100
3	4	214/216 (99%)	179 (84%)	34 (16%)	1 (0%)	29	61
3	8	214/216 (99%)	179 (84%)	35 (16%)	0	100	100
3	9	214/216 (99%)	176 (82%)	38 (18%)	0	100	100
3	A	214/216 (99%)	181 (85%)	33 (15%)	0	100	100
3	B	214/216 (99%)	176 (82%)	38 (18%)	0	100	100
3	F	214/216 (99%)	180 (84%)	34 (16%)	0	100	100
3	G	214/216 (99%)	178 (83%)	36 (17%)	0	100	100
3	K	214/216 (99%)	182 (85%)	32 (15%)	0	100	100
3	L	214/216 (99%)	179 (84%)	35 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	214/216 (99%)	180 (84%)	34 (16%)	0	100	100
3	Q	214/216 (99%)	176 (82%)	38 (18%)	0	100	100
3	U	214/216 (99%)	181 (85%)	33 (15%)	0	100	100
3	V	214/216 (99%)	180 (84%)	34 (16%)	0	100	100
3	Z	214/216 (99%)	180 (84%)	34 (16%)	0	100	100
3	a	214/216 (99%)	178 (83%)	36 (17%)	0	100	100
3	e	214/216 (99%)	181 (85%)	33 (15%)	0	100	100
3	f	214/216 (99%)	179 (84%)	35 (16%)	0	100	100
3	j	214/216 (99%)	182 (85%)	32 (15%)	0	100	100
3	k	214/216 (99%)	177 (83%)	37 (17%)	0	100	100
3	o	214/216 (99%)	180 (84%)	34 (16%)	0	100	100
3	p	214/216 (99%)	174 (81%)	40 (19%)	0	100	100
3	t	214/216 (99%)	179 (84%)	35 (16%)	0	100	100
3	u	214/216 (99%)	179 (84%)	35 (16%)	0	100	100
3	y	214/216 (99%)	179 (84%)	35 (16%)	0	100	100
3	z	214/216 (99%)	176 (82%)	38 (18%)	0	100	100
All	All	6968/11050 (63%)	5957 (86%)	1000 (14%)	11 (0%)	50	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	180	ASN
3	4	210	PRO
1	N	180	ASN
1	1	180	ASN
1	6	180	ASN
1	D	180	ASN
1	m	180	ASN
1	r	180	ASN
1	w	180	ASN
1	S	180	ASN
1	h	180	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	51/168 (30%)	51 (100%)	0	100	100
1	1	40/168 (24%)	34 (85%)	6 (15%)	3	12
1	5	51/168 (30%)	51 (100%)	0	100	100
1	6	40/168 (24%)	35 (88%)	5 (12%)	4	17
1	AA	40/168 (24%)	35 (88%)	5 (12%)	4	17
1	AB	51/168 (30%)	51 (100%)	0	100	100
1	C	51/168 (30%)	51 (100%)	0	100	100
1	D	40/168 (24%)	34 (85%)	6 (15%)	3	12
1	H	51/168 (30%)	51 (100%)	0	100	100
1	I	40/168 (24%)	36 (90%)	4 (10%)	7	27
1	M	51/168 (30%)	51 (100%)	0	100	100
1	N	40/168 (24%)	35 (88%)	5 (12%)	4	17
1	R	51/168 (30%)	51 (100%)	0	100	100
1	S	40/168 (24%)	35 (88%)	5 (12%)	4	17
1	W	51/168 (30%)	51 (100%)	0	100	100
1	X	40/168 (24%)	36 (90%)	4 (10%)	7	27
1	b	51/168 (30%)	51 (100%)	0	100	100
1	c	40/168 (24%)	36 (90%)	4 (10%)	7	27
1	g	51/168 (30%)	51 (100%)	0	100	100
1	h	40/168 (24%)	35 (88%)	5 (12%)	4	17
1	l	51/168 (30%)	51 (100%)	0	100	100
1	m	40/168 (24%)	34 (85%)	6 (15%)	3	12
1	q	51/168 (30%)	51 (100%)	0	100	100
1	r	40/168 (24%)	35 (88%)	5 (12%)	4	17
1	v	51/168 (30%)	51 (100%)	0	100	100
1	w	40/168 (24%)	34 (85%)	6 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	9/9 (100%)	9 (100%)	0	100	100
2	7	9/9 (100%)	9 (100%)	0	100	100
2	AC	9/9 (100%)	9 (100%)	0	100	100
2	E	9/9 (100%)	9 (100%)	0	100	100
2	J	9/9 (100%)	9 (100%)	0	100	100
2	O	9/9 (100%)	9 (100%)	0	100	100
2	T	9/9 (100%)	9 (100%)	0	100	100
2	Y	9/9 (100%)	9 (100%)	0	100	100
2	d	9/9 (100%)	9 (100%)	0	100	100
2	i	9/9 (100%)	9 (100%)	0	100	100
2	n	9/9 (100%)	9 (100%)	0	100	100
2	s	9/9 (100%)	9 (100%)	0	100	100
2	x	9/9 (100%)	9 (100%)	0	100	100
3	3	172/172 (100%)	172 (100%)	0	100	100
3	4	172/172 (100%)	170 (99%)	2 (1%)	71	85
3	8	172/172 (100%)	172 (100%)	0	100	100
3	9	172/172 (100%)	172 (100%)	0	100	100
3	A	172/172 (100%)	172 (100%)	0	100	100
3	B	172/172 (100%)	172 (100%)	0	100	100
3	F	172/172 (100%)	172 (100%)	0	100	100
3	G	172/172 (100%)	172 (100%)	0	100	100
3	K	172/172 (100%)	172 (100%)	0	100	100
3	L	172/172 (100%)	172 (100%)	0	100	100
3	P	172/172 (100%)	172 (100%)	0	100	100
3	Q	172/172 (100%)	172 (100%)	0	100	100
3	U	172/172 (100%)	170 (99%)	2 (1%)	71	85
3	V	172/172 (100%)	172 (100%)	0	100	100
3	Z	172/172 (100%)	172 (100%)	0	100	100
3	a	172/172 (100%)	172 (100%)	0	100	100
3	e	172/172 (100%)	172 (100%)	0	100	100
3	f	172/172 (100%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	j	172/172 (100%)	171 (99%)	1 (1%)	86	94
3	k	172/172 (100%)	170 (99%)	2 (1%)	71	85
3	o	172/172 (100%)	172 (100%)	0	100	100
3	p	172/172 (100%)	172 (100%)	0	100	100
3	t	172/172 (100%)	172 (100%)	0	100	100
3	u	172/172 (100%)	172 (100%)	0	100	100
3	y	172/172 (100%)	172 (100%)	0	100	100
3	z	172/172 (100%)	172 (100%)	0	100	100
All	All	5772/8957 (64%)	5699 (99%)	73 (1%)	70	84

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	166	GLN
1	AA	179	ASP
1	AA	188	VAL
1	AA	196	ASP
1	AA	199	LEU
1	1	166	GLN
1	1	179	ASP
1	1	180	ASN
1	1	188	VAL
1	1	196	ASP
1	1	199	LEU
3	4	209	LYS
3	4	210	PRO
1	6	166	GLN
1	6	179	ASP
1	6	188	VAL
1	6	196	ASP
1	6	199	LEU
1	D	166	GLN
1	D	179	ASP
1	D	180	ASN
1	D	188	VAL
1	D	196	ASP
1	D	199	LEU
1	I	166	GLN
1	I	188	VAL

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Mol	Chain	Res	Type
1	I	196	ASP
1	I	199	LEU
1	N	166	GLN
1	N	179	ASP
1	N	188	VAL
1	N	196	ASP
1	N	199	LEU
1	S	166	GLN
1	S	179	ASP
1	S	188	VAL
1	S	196	ASP
1	S	199	LEU
3	U	70	LYS
3	U	134	GLN
1	X	166	GLN
1	X	188	VAL
1	X	196	ASP
1	X	199	LEU
1	c	166	GLN
1	c	188	VAL
1	c	196	ASP
1	c	199	LEU
1	h	166	GLN
1	h	179	ASP
1	h	188	VAL
1	h	196	ASP
1	h	199	LEU
3	j	134	GLN
3	k	117	MET
3	k	178	LYS
1	m	166	GLN
1	m	179	ASP
1	m	180	ASN
1	m	188	VAL
1	m	196	ASP
1	m	199	LEU
1	r	166	GLN
1	r	179	ASP
1	r	188	VAL
1	r	196	ASP
1	r	199	LEU
1	w	166	GLN

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Mol	Chain	Res	Type
1	w	179	ASP
1	w	180	ASN
1	w	188	VAL
1	w	196	ASP
1	w	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	8	134	GLN
3	9	34	GLN
3	A	134	GLN
3	B	34	GLN
3	F	134	GLN
3	G	34	GLN
3	K	134	GLN
3	L	34	GLN
1	N	184	GLN
3	P	134	GLN
3	Q	34	GLN
3	Q	48	ASN
3	V	34	GLN
1	W	159	HIS
3	a	34	GLN
1	c	184	GLN
3	f	34	GLN
3	f	144	ASN
1	h	184	GLN
3	k	34	GLN
3	o	134	GLN
3	u	34	GLN
1	w	184	GLN
3	y	134	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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.

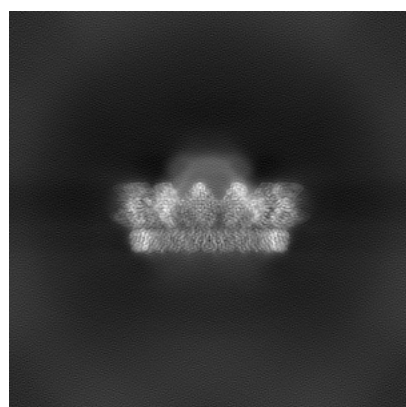
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12963. These allow visual inspection of the internal detail of the map and identification of artifacts.

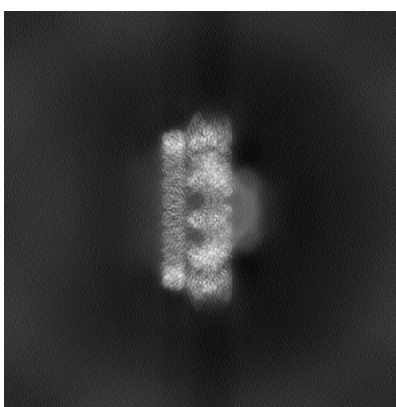
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

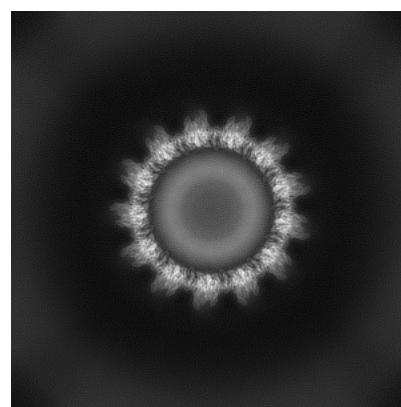
6.1.1 Primary map



X



Y

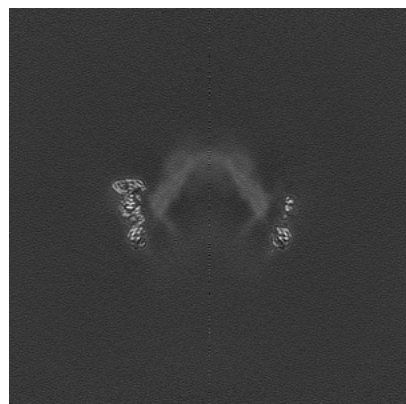


Z

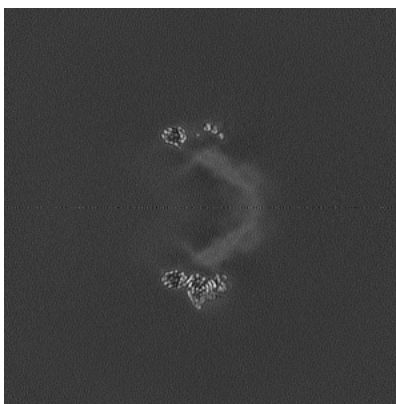
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

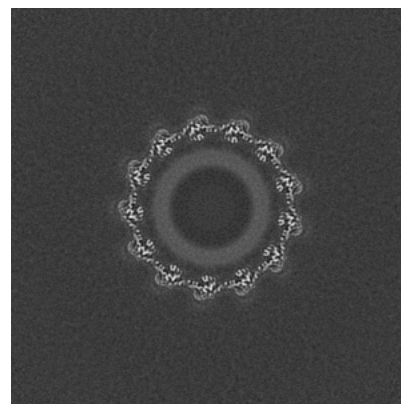
6.2.1 Primary map



X Index: 240



Y Index: 240

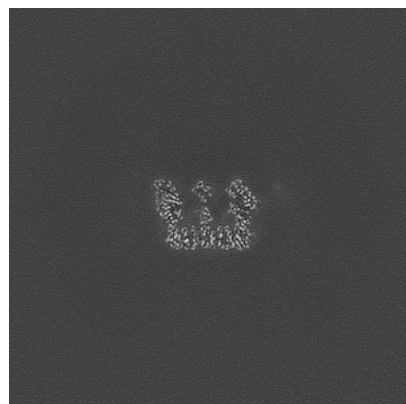


Z Index: 240

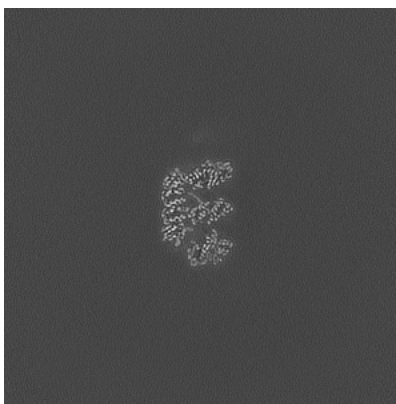
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

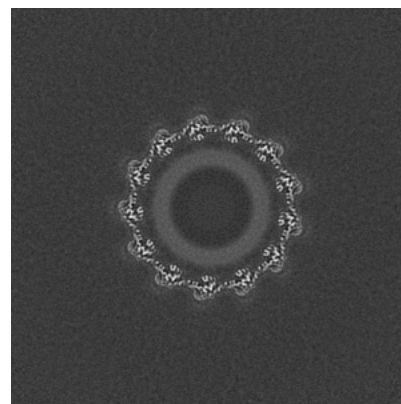
6.3.1 Primary map



X Index: 158



Y Index: 154

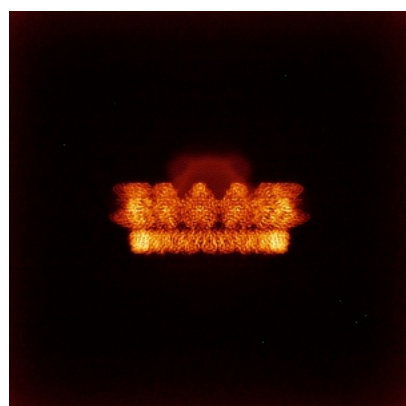


Z Index: 240

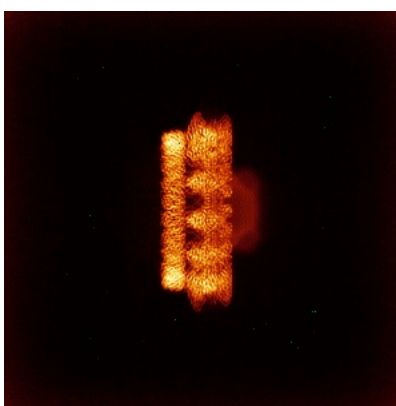
The images above show the largest variance slices of the map in three orthogonal directions.

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

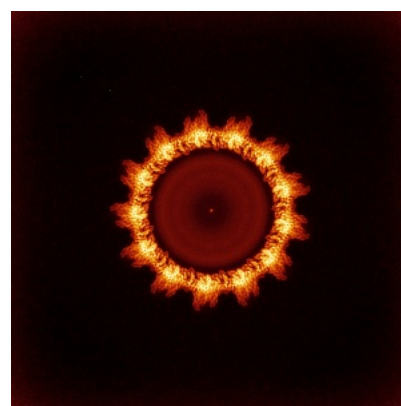
6.4.1 Primary map



X



Y

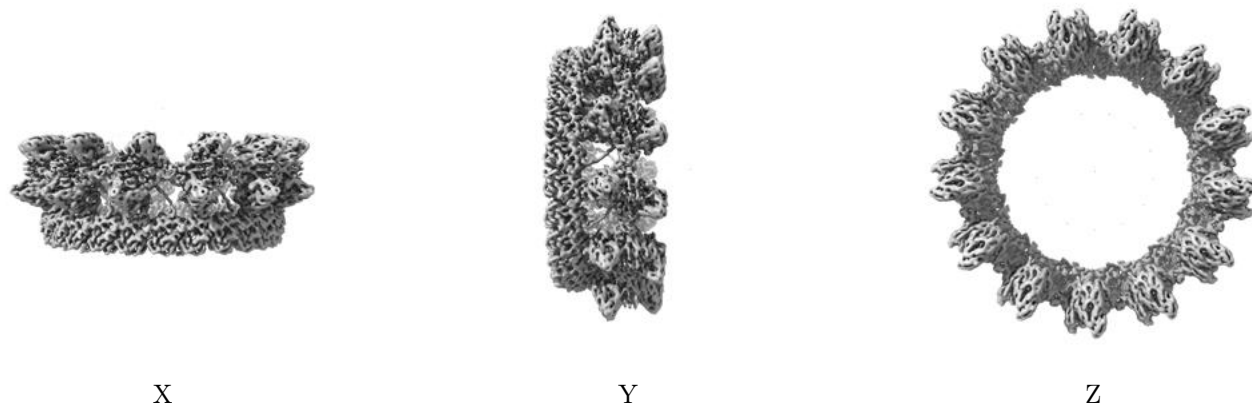


Z

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 0.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

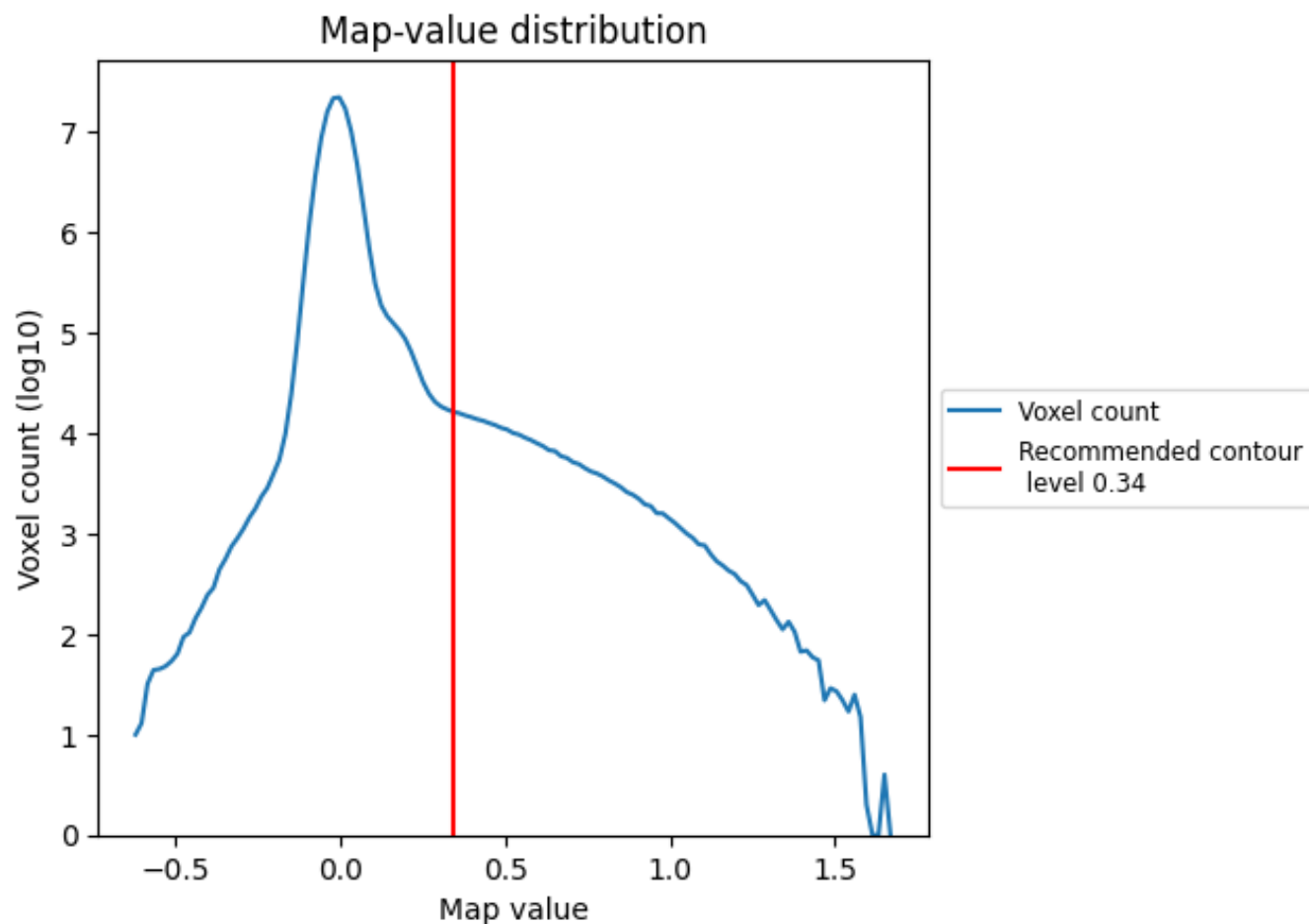
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

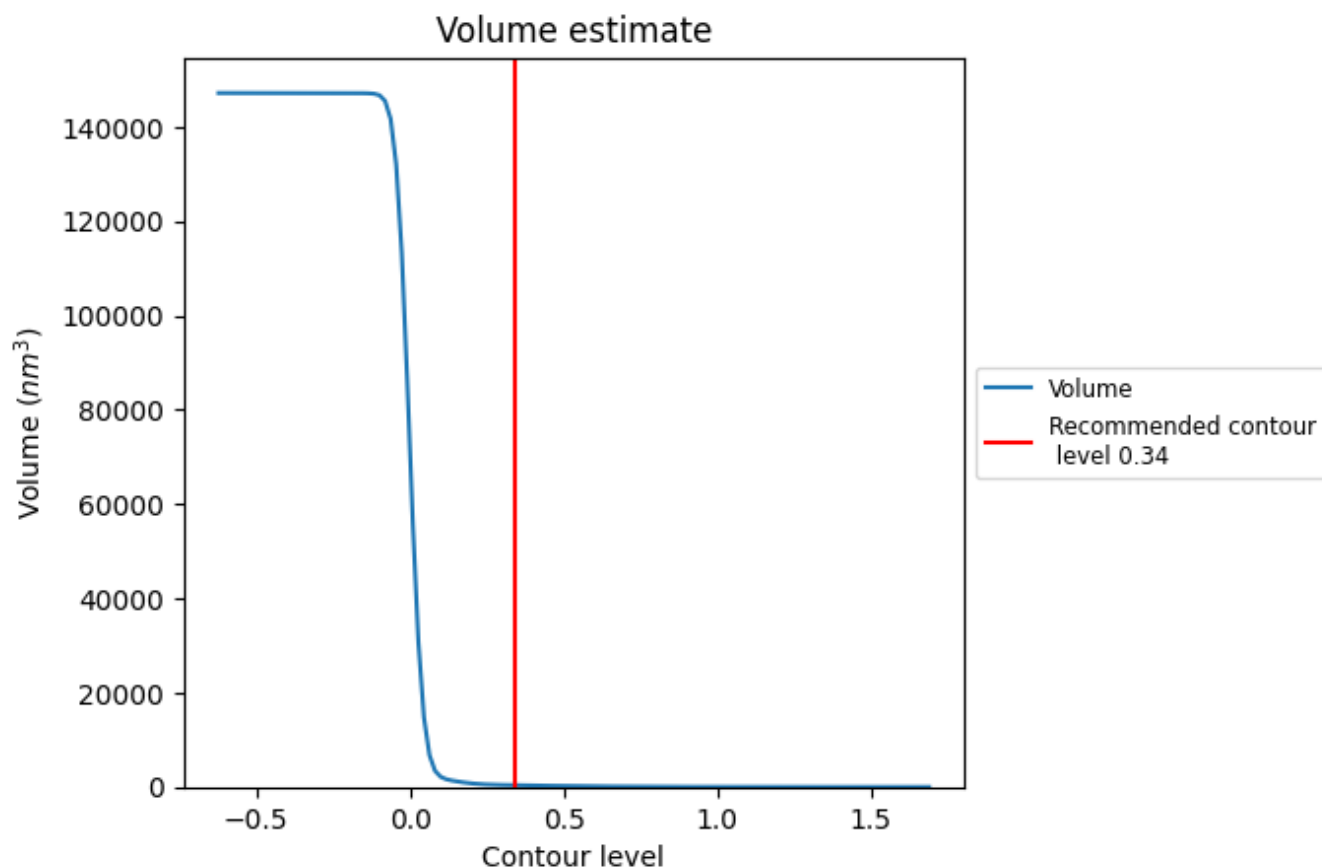
This section contains the results of statistical analysis of the map.

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.

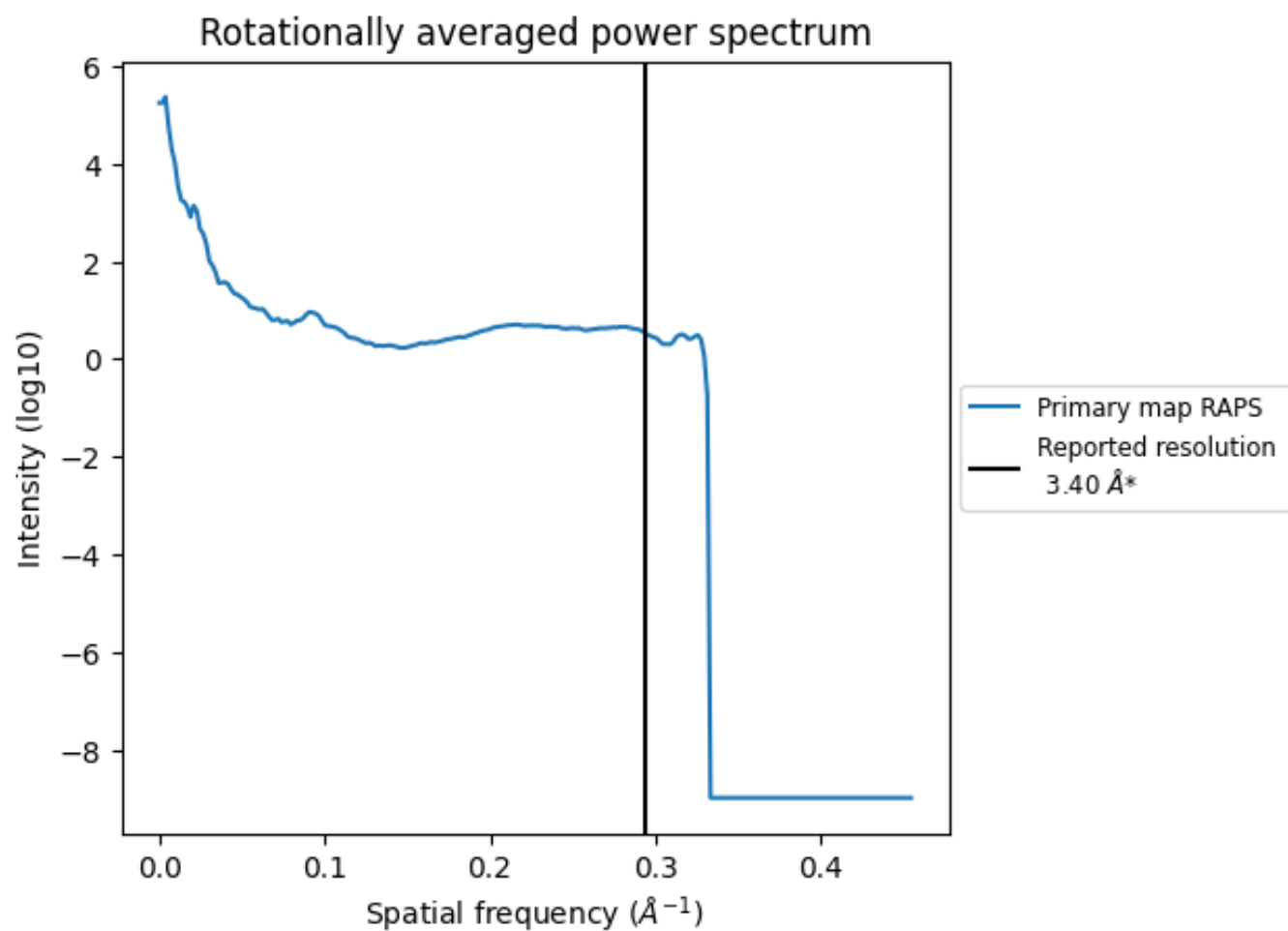
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm^3 ; this corresponds to an approximate mass of 335 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 ⓘ

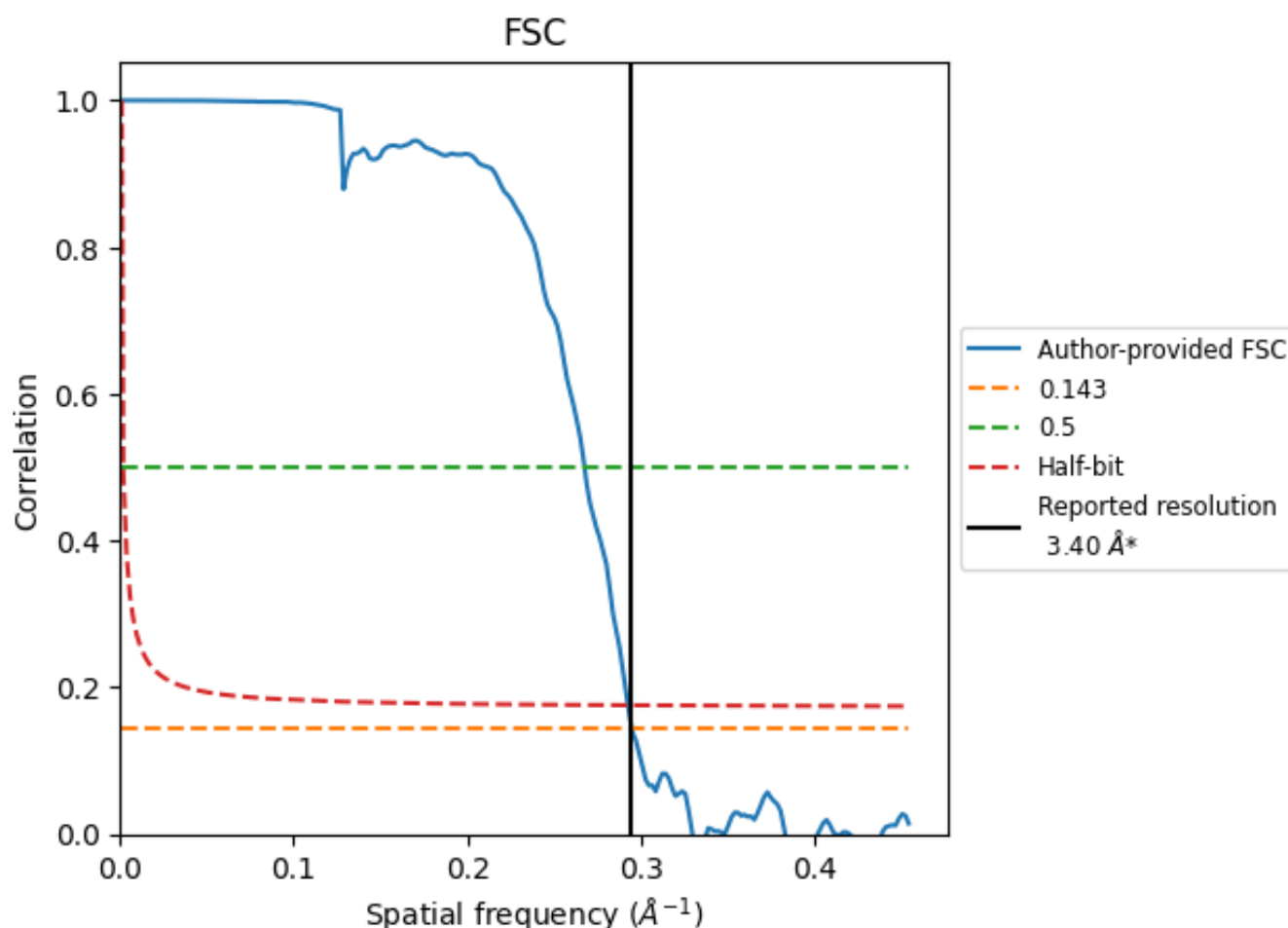


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

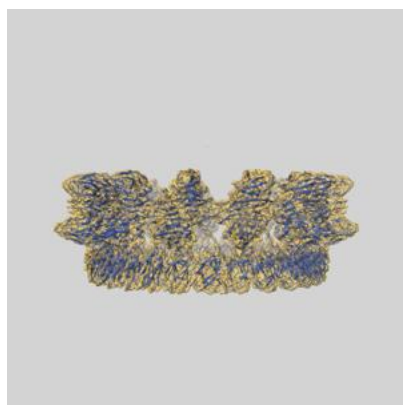
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.74	3.42
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

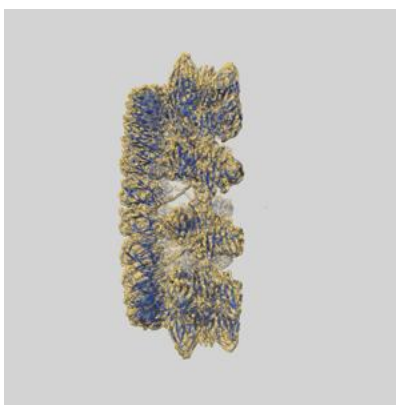
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12963 and PDB model 7OKO. Per-residue inclusion information can be found in section [3](#) on page [10](#).

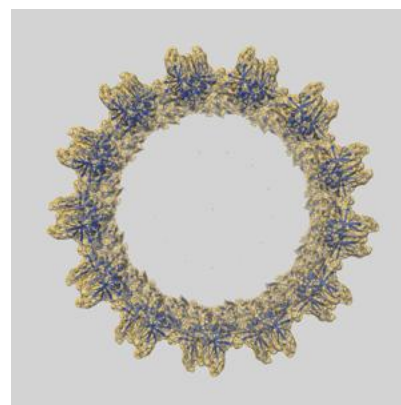
9.1 Map-model overlay [i](#)



X



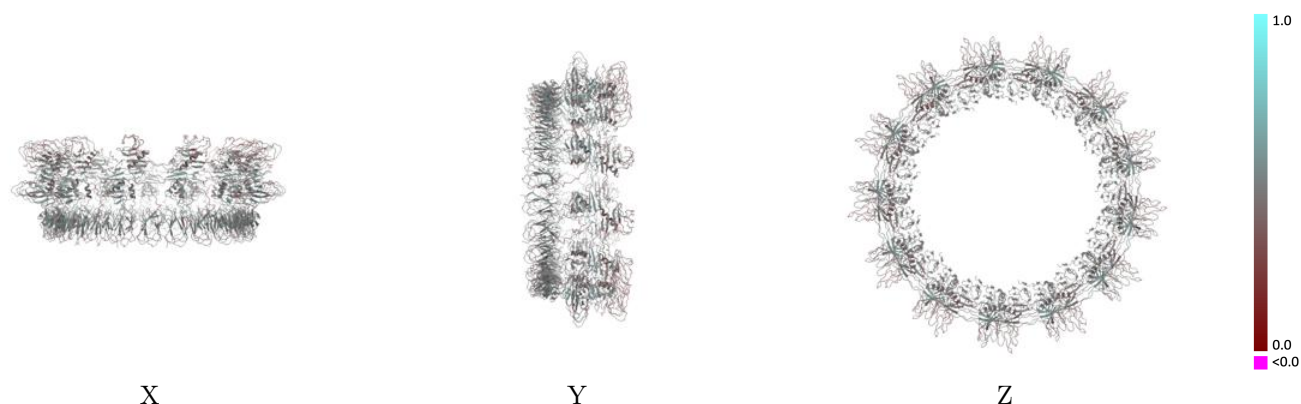
Y



Z

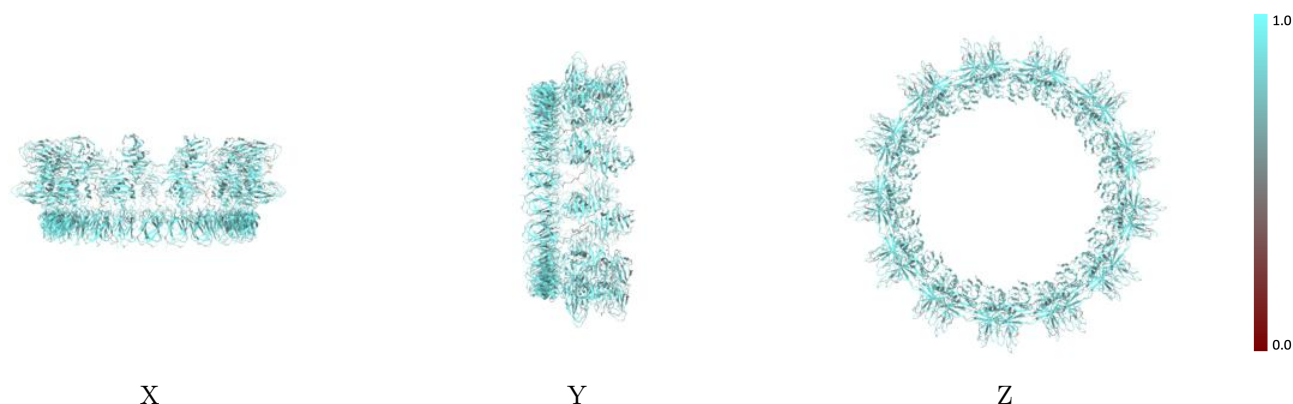
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



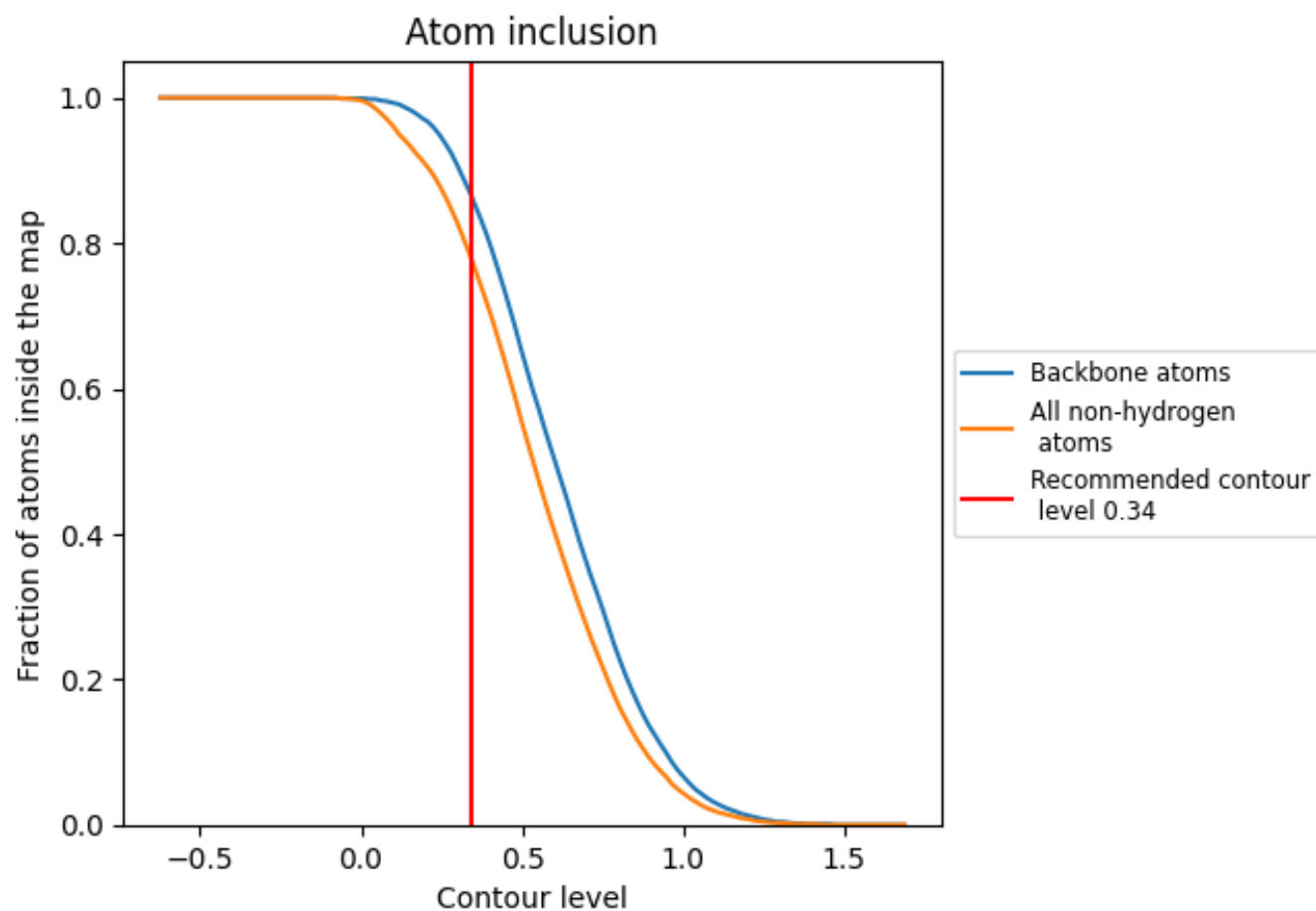
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.34).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.4580
0	 0.7910	 0.4680
1	 0.8110	 0.4890
2	 0.7370	 0.4890
3	 0.8160	 0.4770
4	 0.7430	 0.4300
5	 0.7710	 0.4760
6	 0.8190	 0.4970
7	 0.7240	 0.4860
8	 0.8220	 0.4800
9	 0.7500	 0.4360
A	 0.8210	 0.4810
AA	 0.8250	 0.4990
AB	 0.7930	 0.4700
AC	 0.7370	 0.4850
B	 0.7520	 0.4360
C	 0.7930	 0.4670
D	 0.8160	 0.4960
E	 0.6970	 0.4890
F	 0.8120	 0.4770
G	 0.7360	 0.4290
H	 0.7690	 0.4650
I	 0.8190	 0.4910
J	 0.6970	 0.4850
K	 0.8100	 0.4760
L	 0.7400	 0.4290
M	 0.7580	 0.4660
N	 0.8160	 0.4930
O	 0.6970	 0.4910
P	 0.8190	 0.4780
Q	 0.7450	 0.4330
R	 0.7930	 0.4630
S	 0.8130	 0.4940
T	 0.7110	 0.4790
U	 0.8190	 0.4770



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Chain	Atom inclusion	Q-score
V	 0.7460	 0.4280
W	 0.7750	 0.4590
X	 0.8130	 0.4880
Y	 0.7110	 0.4750
Z	 0.8110	 0.4690
a	 0.7290	 0.4160
b	 0.7510	 0.4420
c	 0.8300	 0.4840
d	 0.7240	 0.4740
e	 0.8140	 0.4730
f	 0.7400	 0.4310
g	 0.7800	 0.4740
h	 0.8190	 0.4790
i	 0.7370	 0.4760
j	 0.8150	 0.4740
k	 0.7320	 0.4240
l	 0.7840	 0.4720
m	 0.8160	 0.4870
n	 0.7240	 0.4660
o	 0.8170	 0.4750
p	 0.7490	 0.4340
q	 0.7840	 0.4770
r	 0.8190	 0.4940
s	 0.6970	 0.4850
t	 0.8140	 0.4760
u	 0.7360	 0.4270
v	 0.7710	 0.4630
w	 0.8160	 0.4890
x	 0.7110	 0.4750
y	 0.8170	 0.4760
z	 0.7540	 0.4370