Full wwPDB EM Validation Report ⓘ

Apr 3, 2024 – 08:56 PM JST

PDB ID	:	8KEC
EMDB ID	:	EMD-37152
Title	:	Cyanophage A-1(L) tail fiber
Authors	:	Yu, R.C.; Li, Q.; Zhou, C.Z.
Deposited on	:	2023-08-11
Resolution	:	3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

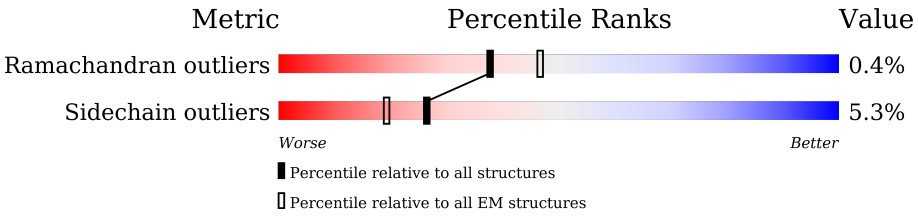
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	A	379	96%
1	B	379	96%
1	C	379	96%
1	D	379	97%
1	E	379	96%
1	F	379	96%
1	G	379	96%
1	H	379	96%
1	I	379	96%

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Mol	Chain	Length	Quality of chain
1	J	379	96%
1	K	379	96%
1	L	379	96%
1	M	379	96%
1	N	379	96%
1	O	379	97%
1	P	379	97%
1	Q	379	96%
1	R	379	97%
2	a	462	57% 40%
2	b	462	5% 56% 5% 39%
2	c	462	57% 40%
2	d	462	56% 40%
2	e	462	5% 57% 39%
2	f	462	58% 40%
2	g	462	56% 40%
2	h	462	5% 57% 39%
2	i	462	57% 40%
2	j	462	56% 5% 40%
2	k	462	5% 56% 5% 39%
2	l	462	57% 40%
2	m	462	57% 40%
2	n	462	5% 55% 5% 39%
2	o	462	57% 40%
2	p	462	57% 40%

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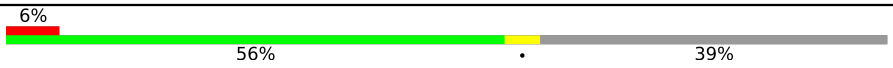
Mol	Chain	Length	Quality of chain
2	q	462	
2	r	462	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 87756 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 Long tail fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	B	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	C	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	D	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	E	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	F	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	G	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	H	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	I	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	J	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	K	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	L	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	M	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	N	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	O	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	P	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	Q	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		

- Molecule 2 is a protein called short tail fiber.

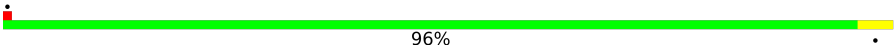
Mol	Chain	Residues	Atoms					AltConf	Trace
2	n	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	i	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	j	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	k	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	l	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	m	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	o	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	p	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	q	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	r	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	a	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	b	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	c	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	d	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	e	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	f	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	g	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	h	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		

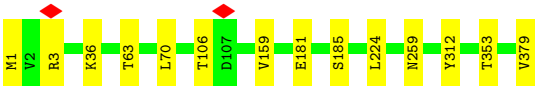
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Long tail fiber

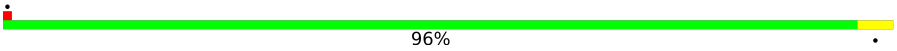
Chain A:

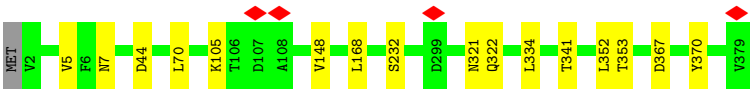




• Molecule 1: Long tail fiber

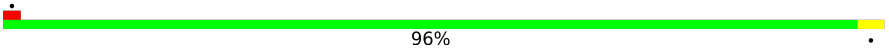
Chain B:

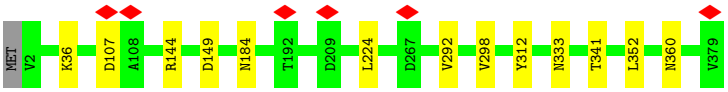




• Molecule 1: Long tail fiber

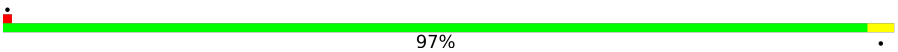
Chain C:

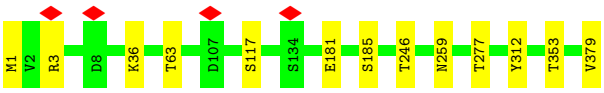




• Molecule 1: Long tail fiber

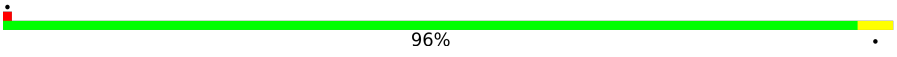
Chain D:

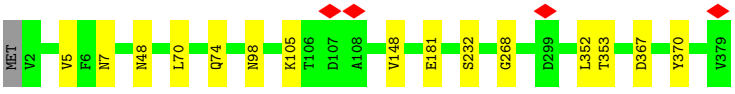




• Molecule 1: Long tail fiber

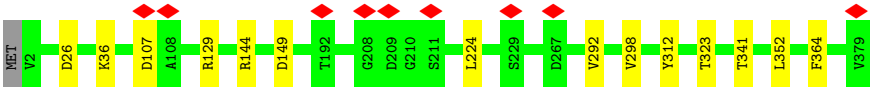
Chain E:





• Molecule 1: Long tail fiber

Chain F:

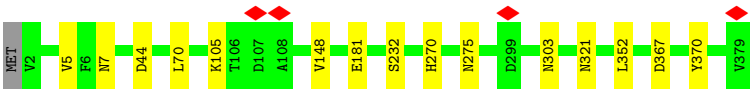


• Molecule 1: Long tail fiber

Chain G:

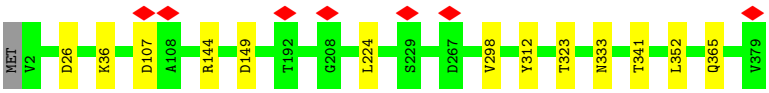
• Molecule 1: Long tail fiber

Chain H:



• Molecule 1: Long tail fiber

Chain I:

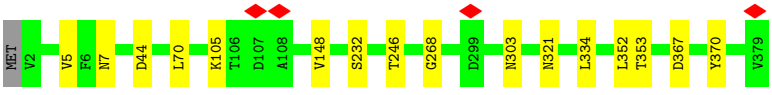


• Molecule 1: Long tail fiber

Chain J:

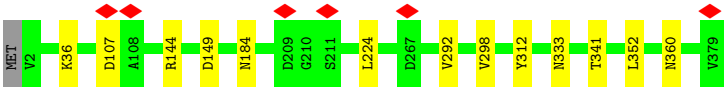
• Molecule 1: Long tail fiber

Chain K:



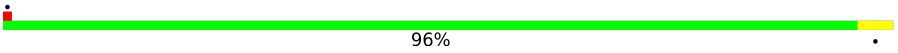
• Molecule 1: Long tail fiber

Chain L:



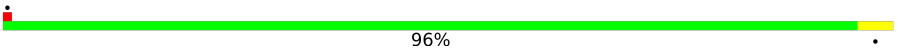
• Molecule 1: Long tail fiber

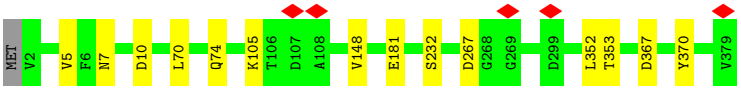
Chain M:



• Molecule 1: Long tail fiber

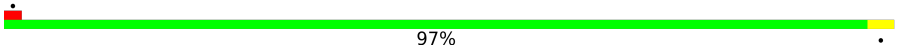
Chain N:

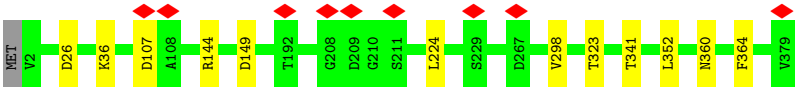




• Molecule 1: Long tail fiber

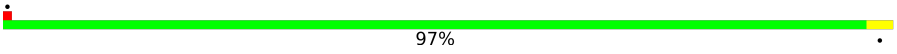
Chain O:

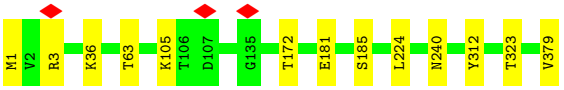




• Molecule 1: Long tail fiber

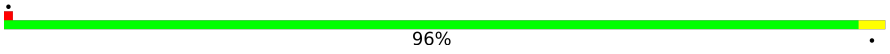
Chain P:

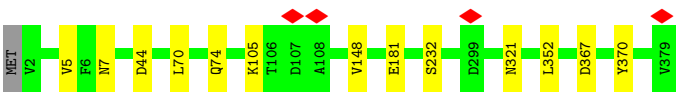




• Molecule 1: Long tail fiber

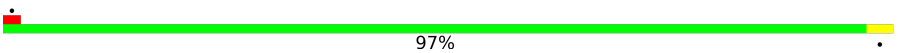
Chain Q:

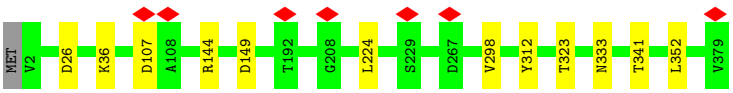




• Molecule 1: Long tail fiber

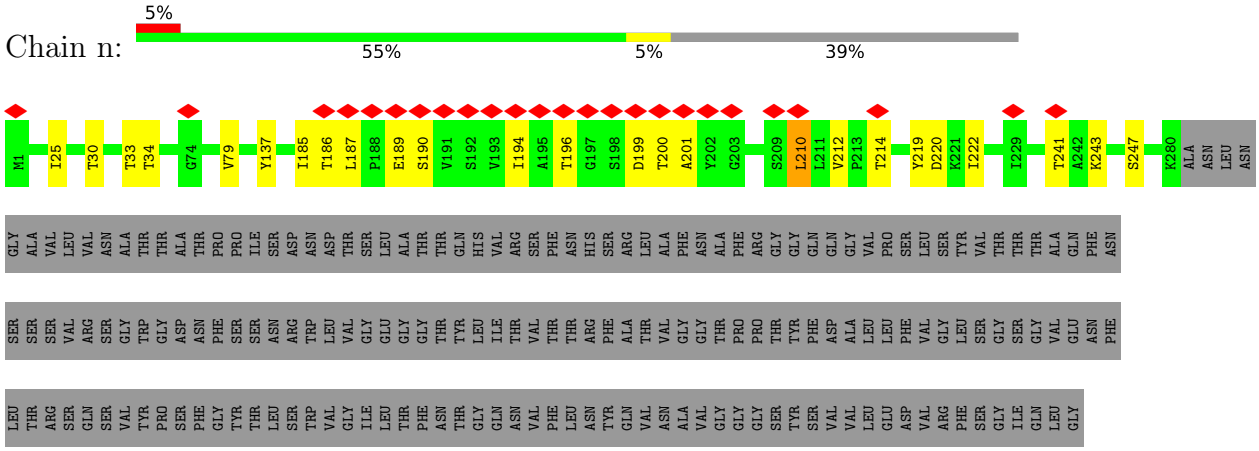
Chain R:





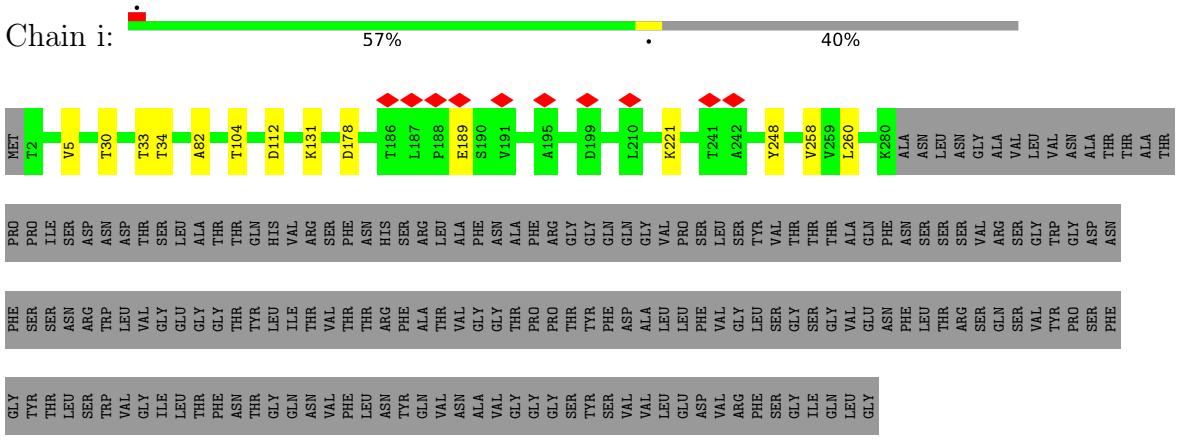
• Molecule 2: short tail fiber

Chain n:



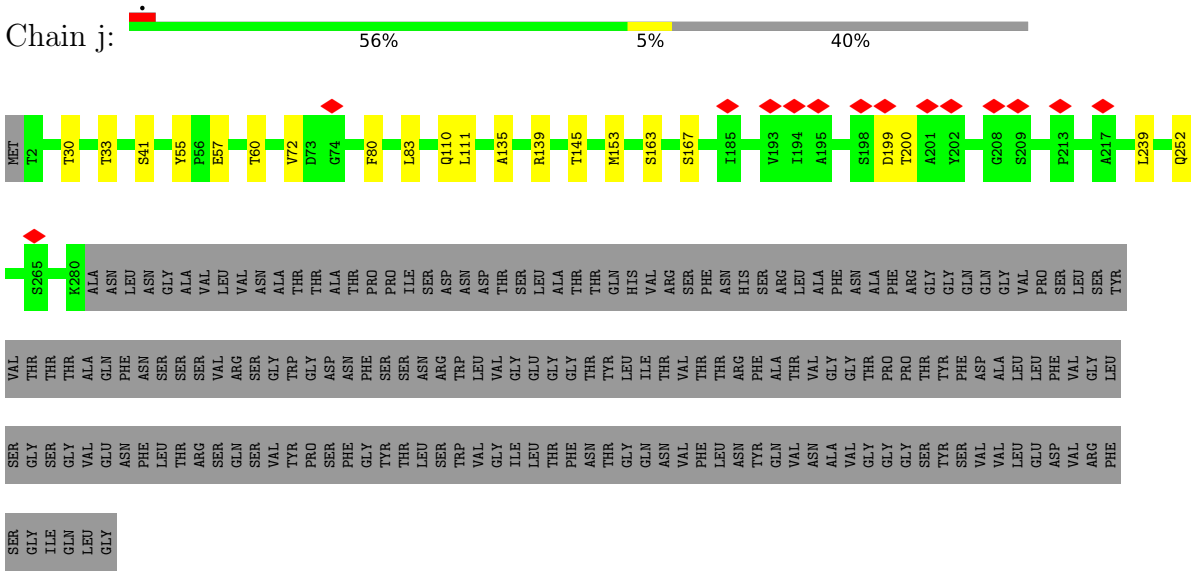
• Molecule 2: short tail fiber

Chain i:



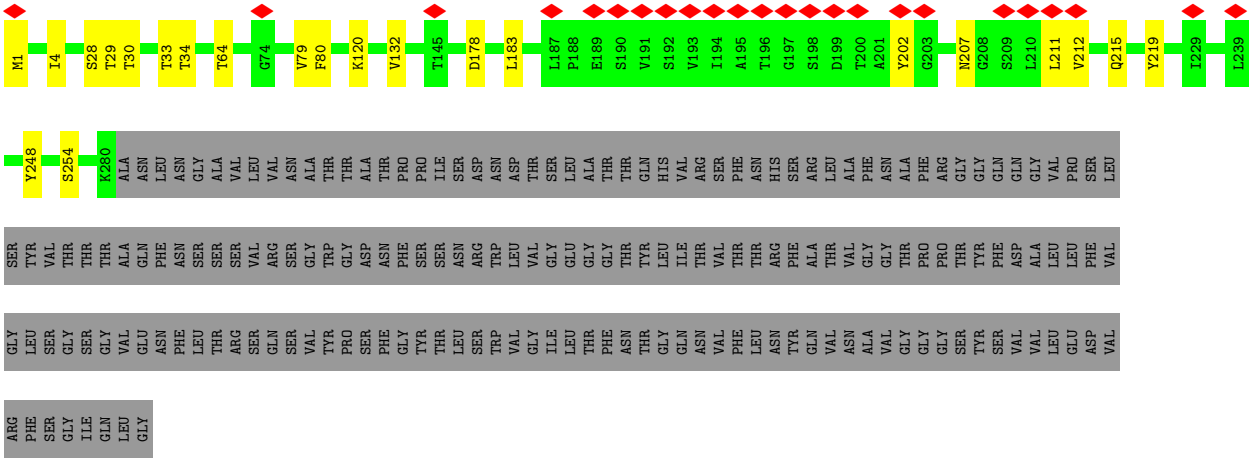
• Molecule 2: short tail fiber

Chain j:



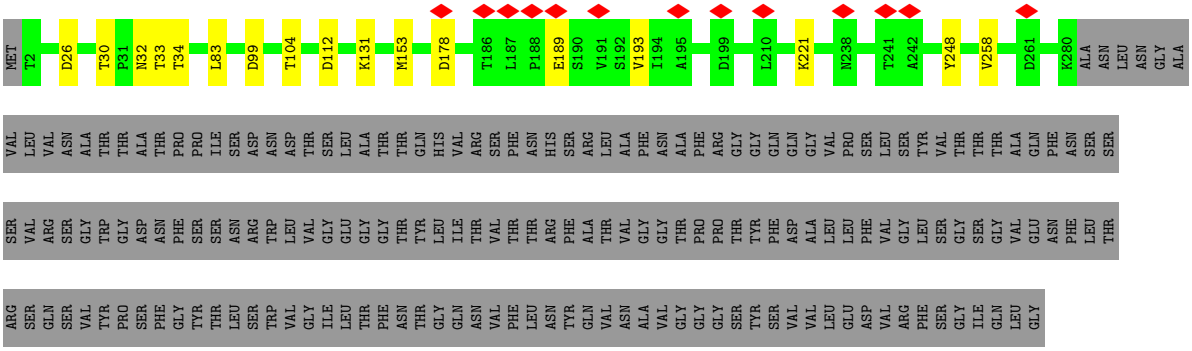
• Molecule 2: short tail fiber

Chain k:



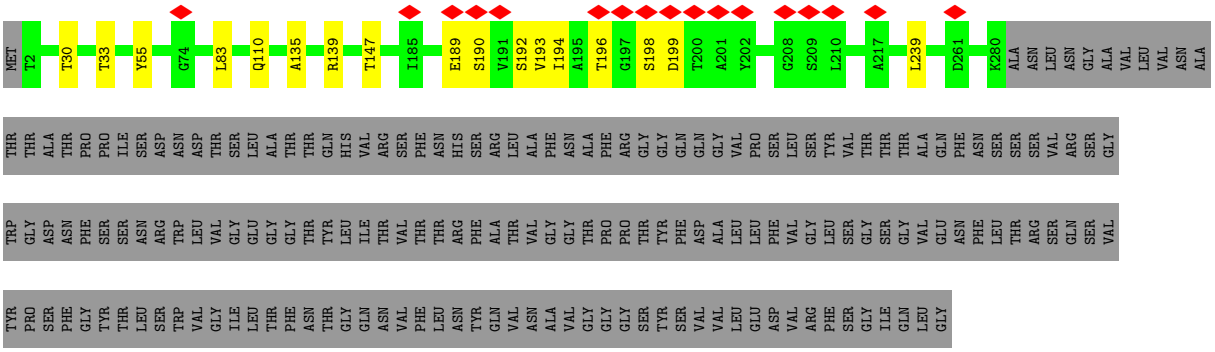
• Molecule 2: short tail fiber

Chain l:



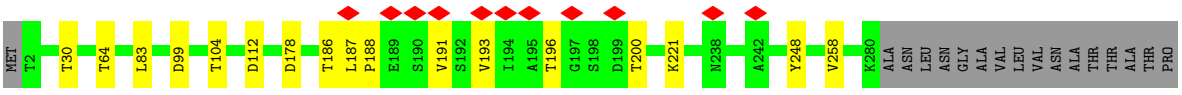
• Molecule 2: short tail fiber

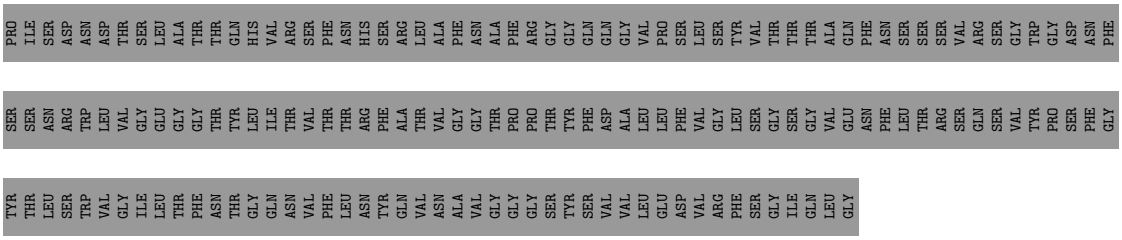
Chain m:



• Molecule 2: short tail fiber

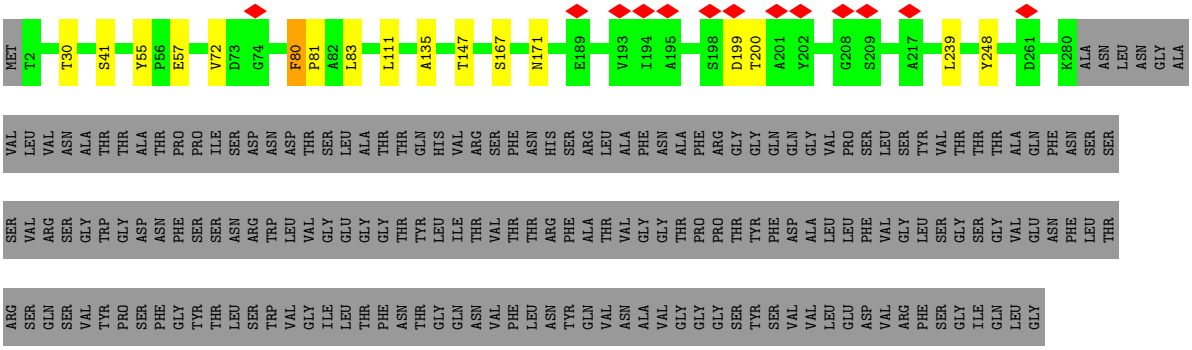
Chain o:





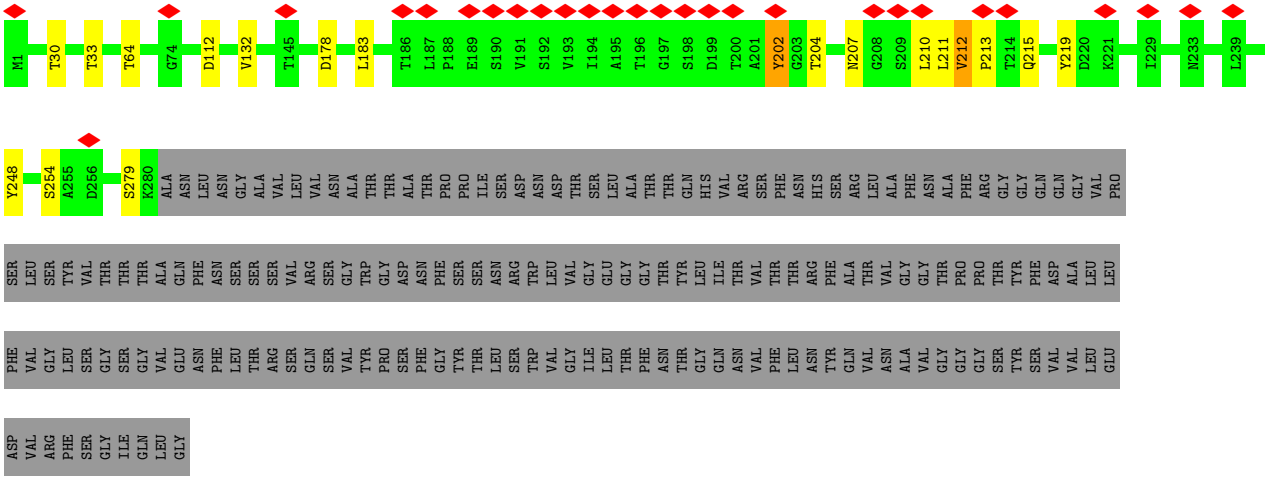
• Molecule 2: short tail fiber

Chain p:



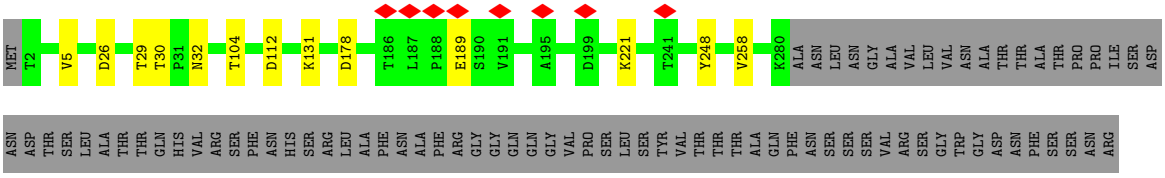
• Molecule 2: short tail fiber

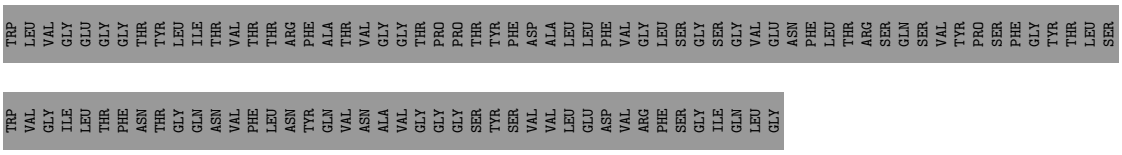
Chain q:



• Molecule 2: short tail fiber

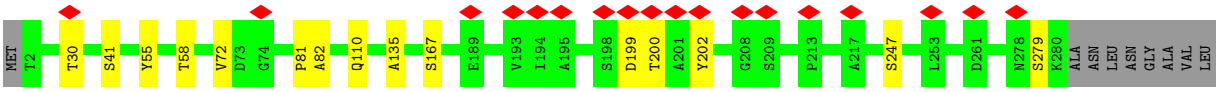
Chain r:

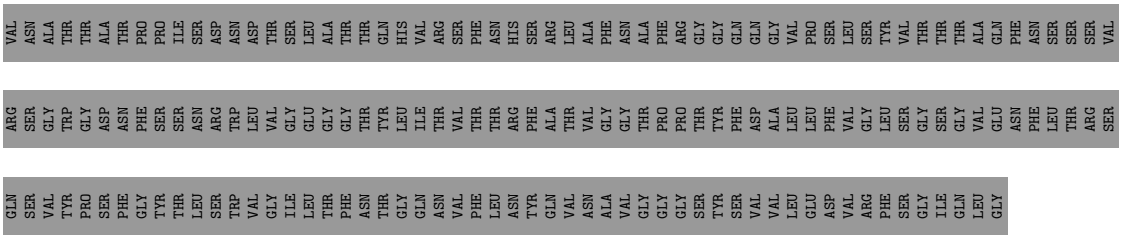




• Molecule 2: short tail fiber

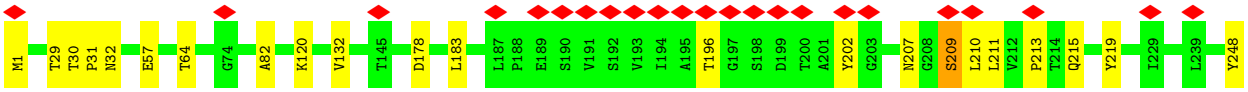
Chain a:

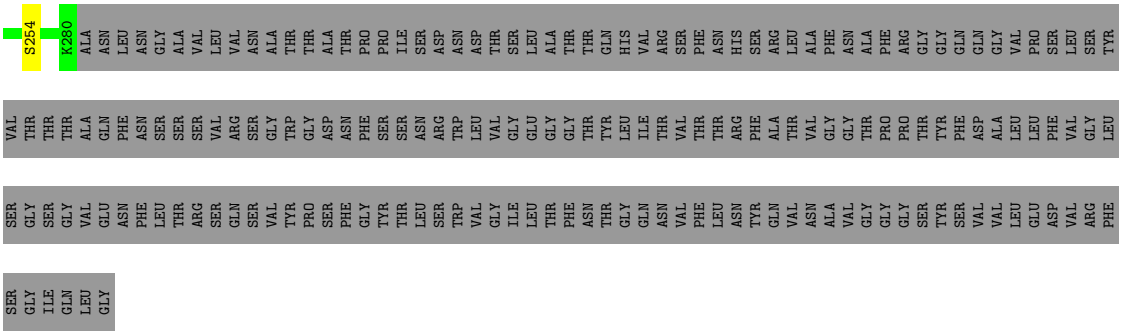




• Molecule 2: short tail fiber

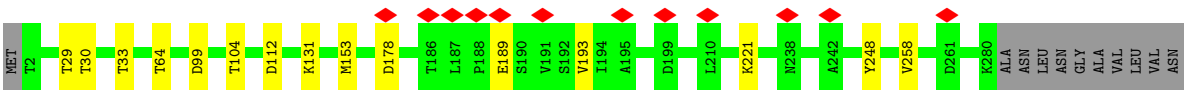
Chain b:

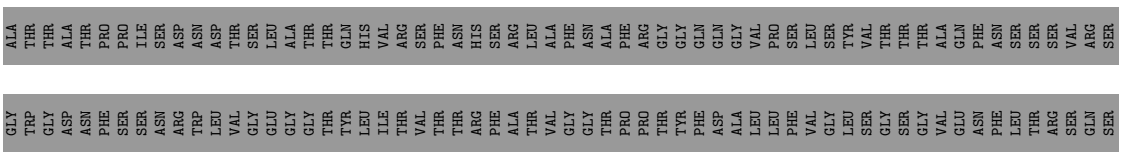




• Molecule 2: short tail fiber

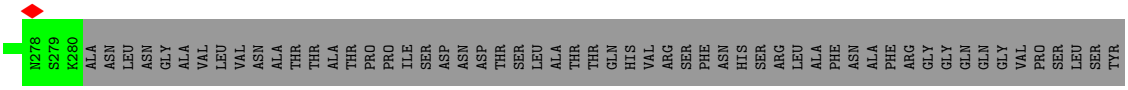
Chain c:





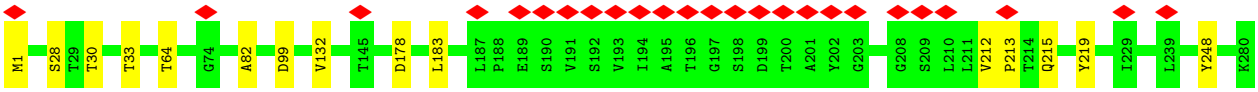
• Molecule 2: short tail fiber

Chain d:



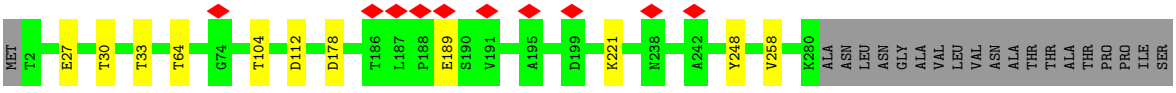
• Molecule 2: short tail fiber

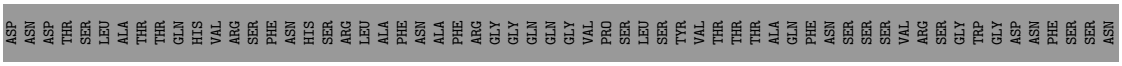
Chain e:



• Molecule 2: short tail fiber

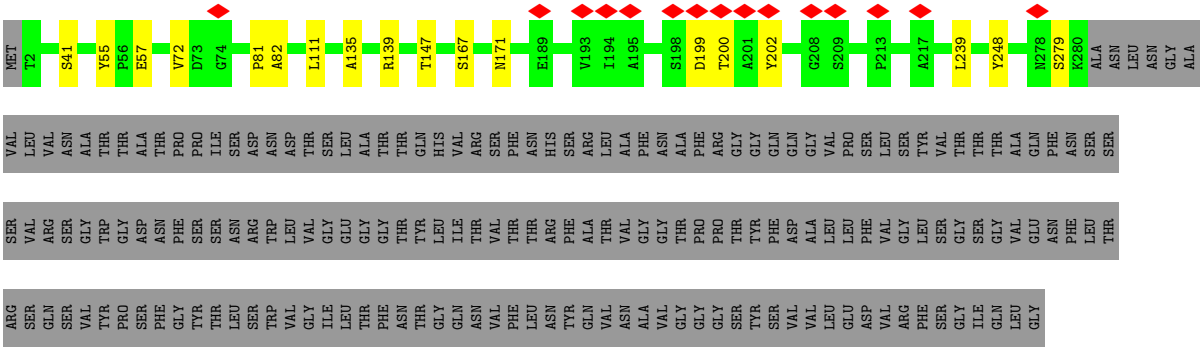
Chain f:





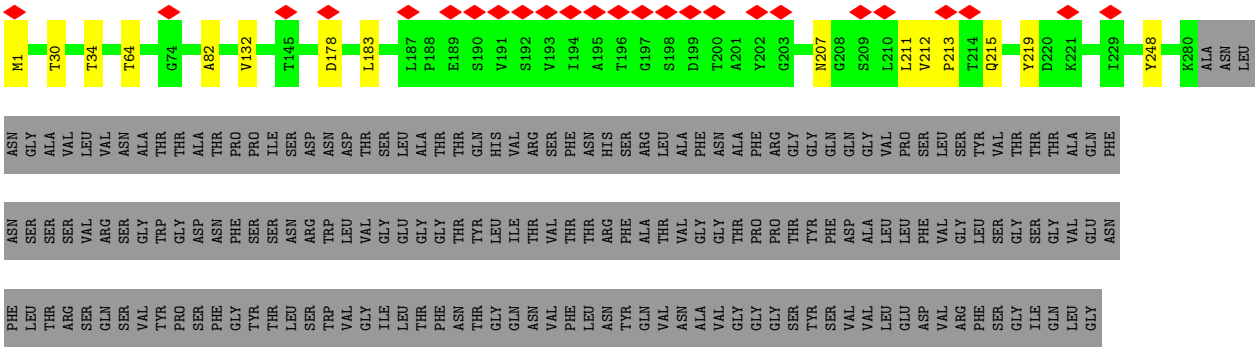
• Molecule 2: short tail fiber

Chain g:



• Molecule 2: short tail fiber

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	A	0.28	0/2859	0.49	0/3916
1	B	0.29	0/2851	0.50	0/3906
1	C	0.28	0/2851	0.50	0/3906
1	D	0.28	0/2859	0.49	0/3916
1	E	0.29	0/2851	0.51	0/3906
1	F	0.29	0/2851	0.51	0/3906
1	G	0.29	0/2859	0.49	0/3916
1	H	0.29	0/2851	0.50	0/3906
1	I	0.28	0/2851	0.50	0/3906
1	J	0.28	0/2859	0.50	0/3916
1	K	0.29	0/2851	0.49	0/3906
1	L	0.28	0/2851	0.50	0/3906
1	M	0.29	0/2859	0.49	0/3916
1	N	0.30	0/2851	0.51	0/3906
1	O	0.28	0/2851	0.50	0/3906
1	P	0.28	0/2859	0.49	0/3916
1	Q	0.29	0/2851	0.50	0/3906
1	R	0.28	0/2851	0.51	0/3906
2	a	0.28	0/2122	0.52	0/2914
2	b	0.29	0/2130	0.53	0/2924
2	c	0.30	0/2122	0.51	0/2914
2	d	0.29	0/2122	0.52	0/2914
2	e	0.29	0/2130	0.54	0/2924
2	f	0.29	0/2122	0.50	0/2914
2	g	0.29	0/2122	0.54	0/2914
2	h	0.30	0/2130	0.54	0/2924
2	i	0.30	0/2122	0.52	0/2914
2	j	0.28	0/2122	0.53	1/2914 (0.0%)
2	k	0.29	0/2130	0.53	0/2924
2	l	0.29	0/2122	0.51	0/2914
2	m	0.31	0/2122	0.58	0/2914
2	n	0.27	0/2130	0.55	0/2924
2	o	0.30	0/2122	0.50	0/2914
2	p	0.32	1/2122 (0.0%)	0.54	0/2914

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
2	q	0.29	0/2130	0.53	0/2924
2	r	0.30	0/2122	0.51	0/2914
All	All	0.29	1/89610 (0.0%)	0.51	1/122880 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	p	81	PRO	N-CD	5.95	1.56	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	80	PHE	N-CA-C	5.71	126.42	111.00

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	A	377/379 (100%)	359 (95%)	18 (5%)	0	100	100
1	B	376/379 (99%)	360 (96%)	16 (4%)	0	100	100
1	C	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
1	D	377/379 (100%)	362 (96%)	15 (4%)	0	100	100
1	E	376/379 (99%)	362 (96%)	13 (4%)	1 (0%)	41	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
1	G	377/379 (100%)	362 (96%)	15 (4%)	0	100	100
1	H	376/379 (99%)	362 (96%)	14 (4%)	0	100	100
1	I	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
1	J	377/379 (100%)	360 (96%)	17 (4%)	0	100	100
1	K	376/379 (99%)	361 (96%)	14 (4%)	1 (0%)	41	75
1	L	376/379 (99%)	360 (96%)	16 (4%)	0	100	100
1	M	377/379 (100%)	358 (95%)	19 (5%)	0	100	100
1	N	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
1	O	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
1	P	377/379 (100%)	362 (96%)	15 (4%)	0	100	100
1	Q	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
1	R	376/379 (99%)	360 (96%)	16 (4%)	0	100	100
2	a	277/462 (60%)	254 (92%)	18 (6%)	5 (2%)	8	42
2	b	278/462 (60%)	256 (92%)	18 (6%)	4 (1%)	11	46
2	c	277/462 (60%)	258 (93%)	17 (6%)	2 (1%)	22	60
2	d	277/462 (60%)	254 (92%)	20 (7%)	3 (1%)	14	51
2	e	278/462 (60%)	256 (92%)	20 (7%)	2 (1%)	22	60
2	f	277/462 (60%)	261 (94%)	16 (6%)	0	100	100
2	g	277/462 (60%)	252 (91%)	20 (7%)	5 (2%)	8	42
2	h	278/462 (60%)	254 (91%)	22 (8%)	2 (1%)	22	60
2	i	277/462 (60%)	259 (94%)	17 (6%)	1 (0%)	34	71
2	j	277/462 (60%)	253 (91%)	21 (8%)	3 (1%)	14	51
2	k	278/462 (60%)	257 (92%)	21 (8%)	0	100	100
2	l	277/462 (60%)	259 (94%)	17 (6%)	1 (0%)	34	71
2	m	277/462 (60%)	256 (92%)	19 (7%)	2 (1%)	22	60
2	n	278/462 (60%)	256 (92%)	18 (6%)	4 (1%)	11	46
2	o	277/462 (60%)	258 (93%)	18 (6%)	1 (0%)	34	71
2	p	277/462 (60%)	251 (91%)	22 (8%)	4 (1%)	11	46
2	q	278/462 (60%)	256 (92%)	19 (7%)	3 (1%)	14	51
2	r	277/462 (60%)	259 (94%)	17 (6%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11766/15138 (78%)	11103 (94%)	618 (5%)	45 (0%)	38 71

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	m	199	ASP
2	q	213	PRO
2	b	31	PRO
2	b	213	PRO
2	c	30	THR
2	e	213	PRO
2	g	82	ALA
2	h	213	PRO
2	n	201	ALA
2	j	199	ASP
2	p	199	ASP
2	a	82	ALA
2	a	199	ASP
2	d	199	ASP
2	e	82	ALA
2	g	199	ASP
2	h	82	ALA
1	E	268	GLY
2	q	202	TYR
2	r	32	ASN
2	a	81	PRO
2	c	29	THR
2	g	81	PRO
2	n	212	VAL
2	l	32	ASN
2	b	82	ALA
2	n	210	LEU
2	i	82	ALA
2	p	200	THR
2	q	212	VAL
2	j	200	THR
2	p	80	PHE
2	a	200	THR
2	b	209	SER
2	d	200	THR
2	g	200	THR
2	j	135	ALA

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Mol	Chain	Res	Type
2	m	135	ALA
2	g	135	ALA
1	K	268	GLY
2	o	188	PRO
2	p	135	ALA
2	a	135	ALA
2	d	135	ALA
2	n	185	ILE

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	A	311/311 (100%)	297 (96%)	14 (4%)	27	56
1	B	310/311 (100%)	294 (95%)	16 (5%)	23	53
1	C	310/311 (100%)	297 (96%)	13 (4%)	30	57
1	D	311/311 (100%)	298 (96%)	13 (4%)	30	57
1	E	310/311 (100%)	296 (96%)	14 (4%)	27	56
1	F	310/311 (100%)	296 (96%)	14 (4%)	27	56
1	G	311/311 (100%)	296 (95%)	15 (5%)	25	54
1	H	310/311 (100%)	295 (95%)	15 (5%)	25	54
1	I	310/311 (100%)	297 (96%)	13 (4%)	30	57
1	J	311/311 (100%)	295 (95%)	16 (5%)	24	53
1	K	310/311 (100%)	295 (95%)	15 (5%)	25	54
1	L	310/311 (100%)	297 (96%)	13 (4%)	30	57
1	M	311/311 (100%)	297 (96%)	14 (4%)	27	56
1	N	310/311 (100%)	296 (96%)	14 (4%)	27	56
1	O	310/311 (100%)	298 (96%)	12 (4%)	32	59
1	P	311/311 (100%)	298 (96%)	13 (4%)	30	57
1	Q	310/311 (100%)	297 (96%)	13 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	310/311 (100%)	298 (96%)	12 (4%)	32 59
2	a	234/384 (61%)	224 (96%)	10 (4%)	29 57
2	b	235/384 (61%)	215 (92%)	20 (8%)	10 39
2	c	234/384 (61%)	221 (94%)	13 (6%)	21 51
2	d	234/384 (61%)	217 (93%)	17 (7%)	14 43
2	e	235/384 (61%)	222 (94%)	13 (6%)	21 51
2	f	234/384 (61%)	223 (95%)	11 (5%)	26 55
2	g	234/384 (61%)	221 (94%)	13 (6%)	21 51
2	h	235/384 (61%)	222 (94%)	13 (6%)	21 51
2	i	234/384 (61%)	221 (94%)	13 (6%)	21 51
2	j	234/384 (61%)	217 (93%)	17 (7%)	14 43
2	k	235/384 (61%)	213 (91%)	22 (9%)	8 33
2	l	234/384 (61%)	218 (93%)	16 (7%)	16 45
2	m	234/384 (61%)	219 (94%)	15 (6%)	17 47
2	n	235/384 (61%)	213 (91%)	22 (9%)	8 33
2	o	234/384 (61%)	218 (93%)	16 (7%)	16 45
2	p	234/384 (61%)	221 (94%)	13 (6%)	21 51
2	q	235/384 (61%)	217 (92%)	18 (8%)	13 42
2	r	234/384 (61%)	222 (95%)	12 (5%)	24 53
All	All	9804/12510 (78%)	9281 (95%)	523 (5%)	26 52

All (523) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ARG
1	A	36	LYS
1	A	63	THR
1	A	70	LEU
1	A	106	THR
1	A	159	VAL
1	A	181	GLU
1	A	185	SER
1	A	224	LEU
1	A	259	ASN

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Mol	Chain	Res	Type
1	A	312	TYR
1	A	353	THR
1	A	379	VAL
1	B	5	VAL
1	B	7	ASN
1	B	44	ASP
1	B	70	LEU
1	B	105	LYS
1	B	148	VAL
1	B	168	LEU
1	B	232	SER
1	B	321	ASN
1	B	322	GLN
1	B	334	LEU
1	B	341	THR
1	B	352	LEU
1	B	353	THR
1	B	367	ASP
1	B	370	TYR
1	C	36	LYS
1	C	107	ASP
1	C	144	ARG
1	C	149	ASP
1	C	184	ASN
1	C	224	LEU
1	C	292	VAL
1	C	298	VAL
1	C	312	TYR
1	C	333	ASN
1	C	341	THR
1	C	352	LEU
1	C	360	ASN
1	D	1	MET
1	D	3	ARG
1	D	36	LYS
1	D	63	THR
1	D	117	SER
1	D	181	GLU
1	D	185	SER
1	D	246	THR
1	D	259	ASN
1	D	277	THR

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Mol	Chain	Res	Type
1	D	312	TYR
1	D	353	THR
1	D	379	VAL
1	E	5	VAL
1	E	7	ASN
1	E	48	ASN
1	E	70	LEU
1	E	74	GLN
1	E	98	ASN
1	E	105	LYS
1	E	148	VAL
1	E	181	GLU
1	E	232	SER
1	E	352	LEU
1	E	353	THR
1	E	367	ASP
1	E	370	TYR
1	F	26	ASP
1	F	36	LYS
1	F	107	ASP
1	F	129	ARG
1	F	144	ARG
1	F	149	ASP
1	F	224	LEU
1	F	292	VAL
1	F	298	VAL
1	F	312	TYR
1	F	323	THR
1	F	341	THR
1	F	352	LEU
1	F	364	PHE
1	G	1	MET
1	G	3	ARG
1	G	63	THR
1	G	105	LYS
1	G	172	THR
1	G	181	GLU
1	G	184	ASN
1	G	185	SER
1	G	224	LEU
1	G	240	ASN
1	G	259	ASN

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Mol	Chain	Res	Type
1	G	312	TYR
1	G	323	THR
1	G	367	ASP
1	G	379	VAL
1	H	5	VAL
1	H	7	ASN
1	H	44	ASP
1	H	70	LEU
1	H	105	LYS
1	H	148	VAL
1	H	181	GLU
1	H	232	SER
1	H	270	HIS
1	H	275	ASN
1	H	303	ASN
1	H	321	ASN
1	H	352	LEU
1	H	367	ASP
1	H	370	TYR
1	I	26	ASP
1	I	36	LYS
1	I	107	ASP
1	I	144	ARG
1	I	149	ASP
1	I	224	LEU
1	I	298	VAL
1	I	312	TYR
1	I	323	THR
1	I	333	ASN
1	I	341	THR
1	I	352	LEU
1	I	365	GLN
1	J	1	MET
1	J	3	ARG
1	J	36	LYS
1	J	63	THR
1	J	70	LEU
1	J	106	THR
1	J	117	SER
1	J	159	VAL
1	J	181	GLU
1	J	185	SER

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Mol	Chain	Res	Type
1	J	224	LEU
1	J	259	ASN
1	J	312	TYR
1	J	353	THR
1	J	367	ASP
1	J	379	VAL
1	K	5	VAL
1	K	7	ASN
1	K	44	ASP
1	K	70	LEU
1	K	105	LYS
1	K	148	VAL
1	K	232	SER
1	K	246	THR
1	K	303	ASN
1	K	321	ASN
1	K	334	LEU
1	K	352	LEU
1	K	353	THR
1	K	367	ASP
1	K	370	TYR
1	L	36	LYS
1	L	107	ASP
1	L	144	ARG
1	L	149	ASP
1	L	184	ASN
1	L	224	LEU
1	L	292	VAL
1	L	298	VAL
1	L	312	TYR
1	L	333	ASN
1	L	341	THR
1	L	352	LEU
1	L	360	ASN
1	M	1	MET
1	M	3	ARG
1	M	36	LYS
1	M	63	THR
1	M	181	GLU
1	M	185	SER
1	M	211	SER
1	M	212	THR

Continued on next page...

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Mol	Chain	Res	Type
1	M	246	THR
1	M	259	ASN
1	M	277	THR
1	M	312	TYR
1	M	353	THR
1	M	379	VAL
1	N	5	VAL
1	N	7	ASN
1	N	10	ASP
1	N	70	LEU
1	N	74	GLN
1	N	105	LYS
1	N	148	VAL
1	N	181	GLU
1	N	232	SER
1	N	267	ASP
1	N	352	LEU
1	N	353	THR
1	N	367	ASP
1	N	370	TYR
1	O	26	ASP
1	O	36	LYS
1	O	107	ASP
1	O	144	ARG
1	O	149	ASP
1	O	224	LEU
1	O	298	VAL
1	O	323	THR
1	O	341	THR
1	O	352	LEU
1	O	360	ASN
1	O	364	PHE
1	P	1	MET
1	P	3	ARG
1	P	36	LYS
1	P	63	THR
1	P	105	LYS
1	P	172	THR
1	P	181	GLU
1	P	185	SER
1	P	224	LEU
1	P	240	ASN

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Mol	Chain	Res	Type
1	P	312	TYR
1	P	323	THR
1	P	379	VAL
1	Q	5	VAL
1	Q	7	ASN
1	Q	44	ASP
1	Q	70	LEU
1	Q	74	GLN
1	Q	105	LYS
1	Q	148	VAL
1	Q	181	GLU
1	Q	232	SER
1	Q	321	ASN
1	Q	352	LEU
1	Q	367	ASP
1	Q	370	TYR
1	R	26	ASP
1	R	36	LYS
1	R	107	ASP
1	R	144	ARG
1	R	149	ASP
1	R	224	LEU
1	R	298	VAL
1	R	312	TYR
1	R	323	THR
1	R	333	ASN
1	R	341	THR
1	R	352	LEU
2	n	25	ILE
2	n	30	THR
2	n	33	THR
2	n	34	THR
2	n	79	VAL
2	n	137	TYR
2	n	186	THR
2	n	187	LEU
2	n	189	GLU
2	n	190	SER
2	n	194	ILE
2	n	196	THR
2	n	199	ASP
2	n	200	THR

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Mol	Chain	Res	Type
2	n	210	LEU
2	n	214	THR
2	n	219	TYR
2	n	220	ASP
2	n	222	ILE
2	n	241	THR
2	n	243	LYS
2	n	247	SER
2	i	5	VAL
2	i	30	THR
2	i	33	THR
2	i	34	THR
2	i	104	THR
2	i	112	ASP
2	i	131	LYS
2	i	178	ASP
2	i	189	GLU
2	i	221	LYS
2	i	248	TYR
2	i	258	VAL
2	i	260	LEU
2	j	30	THR
2	j	33	THR
2	j	41	SER
2	j	55	TYR
2	j	57	GLU
2	j	60	THR
2	j	72	VAL
2	j	83	LEU
2	j	110	GLN
2	j	111	LEU
2	j	139	ARG
2	j	145	THR
2	j	153	MET
2	j	163	SER
2	j	167	SER
2	j	239	LEU
2	j	252	GLN
2	k	1	MET
2	k	4	ILE
2	k	28	SER
2	k	29	THR

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Mol	Chain	Res	Type
2	k	30	THR
2	k	33	THR
2	k	34	THR
2	k	64	THR
2	k	79	VAL
2	k	80	PHE
2	k	120	LYS
2	k	132	VAL
2	k	178	ASP
2	k	183	LEU
2	k	202	TYR
2	k	207	ASN
2	k	211	LEU
2	k	212	VAL
2	k	215	GLN
2	k	219	TYR
2	k	248	TYR
2	k	254	SER
2	l	26	ASP
2	l	30	THR
2	l	33	THR
2	l	34	THR
2	l	83	LEU
2	l	99	ASP
2	l	104	THR
2	l	112	ASP
2	l	131	LYS
2	l	153	MET
2	l	178	ASP
2	l	189	GLU
2	l	193	VAL
2	l	221	LYS
2	l	248	TYR
2	l	258	VAL
2	m	30	THR
2	m	33	THR
2	m	55	TYR
2	m	83	LEU
2	m	110	GLN
2	m	139	ARG
2	m	147	THR
2	m	189	GLU

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Mol	Chain	Res	Type
2	m	190	SER
2	m	192	SER
2	m	193	VAL
2	m	194	ILE
2	m	196	THR
2	m	198	SER
2	m	239	LEU
2	o	30	THR
2	o	64	THR
2	o	83	LEU
2	o	99	ASP
2	o	104	THR
2	o	112	ASP
2	o	178	ASP
2	o	186	THR
2	o	187	LEU
2	o	191	VAL
2	o	193	VAL
2	o	196	THR
2	o	200	THR
2	o	221	LYS
2	o	248	TYR
2	o	258	VAL
2	p	30	THR
2	p	41	SER
2	p	55	TYR
2	p	57	GLU
2	p	72	VAL
2	p	80	PHE
2	p	83	LEU
2	p	111	LEU
2	p	147	THR
2	p	167	SER
2	p	171	ASN
2	p	239	LEU
2	p	248	TYR
2	q	30	THR
2	q	33	THR
2	q	64	THR
2	q	112	ASP
2	q	132	VAL
2	q	178	ASP

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Mol	Chain	Res	Type
2	q	183	LEU
2	q	202	TYR
2	q	204	THR
2	q	207	ASN
2	q	210	LEU
2	q	211	LEU
2	q	212	VAL
2	q	215	GLN
2	q	219	TYR
2	q	248	TYR
2	q	254	SER
2	q	279	SER
2	r	5	VAL
2	r	26	ASP
2	r	29	THR
2	r	30	THR
2	r	104	THR
2	r	112	ASP
2	r	131	LYS
2	r	178	ASP
2	r	189	GLU
2	r	221	LYS
2	r	248	TYR
2	r	258	VAL
2	a	30	THR
2	a	41	SER
2	a	55	TYR
2	a	58	THR
2	a	72	VAL
2	a	110	GLN
2	a	167	SER
2	a	202	TYR
2	a	247	SER
2	a	279	SER
2	b	1	MET
2	b	29	THR
2	b	30	THR
2	b	32	ASN
2	b	57	GLU
2	b	64	THR
2	b	120	LYS
2	b	132	VAL

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Mol	Chain	Res	Type
2	b	178	ASP
2	b	183	LEU
2	b	196	THR
2	b	202	TYR
2	b	207	ASN
2	b	209	SER
2	b	210	LEU
2	b	211	LEU
2	b	215	GLN
2	b	219	TYR
2	b	248	TYR
2	b	254	SER
2	c	33	THR
2	c	64	THR
2	c	99	ASP
2	c	104	THR
2	c	112	ASP
2	c	131	LYS
2	c	153	MET
2	c	178	ASP
2	c	189	GLU
2	c	193	VAL
2	c	221	LYS
2	c	248	TYR
2	c	258	VAL
2	d	41	SER
2	d	55	TYR
2	d	57	GLU
2	d	60	THR
2	d	71	SER
2	d	73	ASP
2	d	76	SER
2	d	80	PHE
2	d	83	LEU
2	d	139	ARG
2	d	147	THR
2	d	153	MET
2	d	163	SER
2	d	167	SER
2	d	202	TYR
2	d	239	LEU
2	d	248	TYR

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Mol	Chain	Res	Type
2	e	1	MET
2	e	28	SER
2	e	30	THR
2	e	33	THR
2	e	64	THR
2	e	99	ASP
2	e	132	VAL
2	e	178	ASP
2	e	183	LEU
2	e	212	VAL
2	e	215	GLN
2	e	219	TYR
2	e	248	TYR
2	f	27	GLU
2	f	30	THR
2	f	33	THR
2	f	64	THR
2	f	104	THR
2	f	112	ASP
2	f	178	ASP
2	f	189	GLU
2	f	221	LYS
2	f	248	TYR
2	f	258	VAL
2	g	41	SER
2	g	55	TYR
2	g	57	GLU
2	g	72	VAL
2	g	111	LEU
2	g	139	ARG
2	g	147	THR
2	g	167	SER
2	g	171	ASN
2	g	202	TYR
2	g	239	LEU
2	g	248	TYR
2	g	279	SER
2	h	1	MET
2	h	30	THR
2	h	34	THR
2	h	64	THR
2	h	132	VAL

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Mol	Chain	Res	Type
2	h	178	ASP
2	h	183	LEU
2	h	207	ASN
2	h	211	LEU
2	h	212	VAL
2	h	215	GLN
2	h	219	TYR
2	h	248	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	362	GLN
1	B	368	GLN
1	C	259	ASN
1	C	270	HIS
1	D	259	ASN
1	E	48	ASN
1	E	321	ASN
1	E	362	GLN
1	E	368	GLN
1	F	259	ASN
1	F	365	GLN
1	G	240	ASN
1	G	241	GLN
1	H	48	ASN
1	H	362	GLN
1	H	368	GLN
1	I	259	ASN
1	I	270	HIS
1	K	362	GLN
1	K	368	GLN
1	L	259	ASN
1	M	240	ASN
1	M	241	GLN
1	N	321	ASN
1	N	362	GLN
1	N	368	GLN
1	O	241	GLN
1	O	259	ASN
1	O	270	HIS
1	O	302	ASN

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Mol	Chain	Res	Type
1	O	365	GLN
1	P	240	ASN
1	P	241	GLN
1	P	259	ASN
1	P	272	HIS
1	Q	48	ASN
1	Q	362	GLN
1	Q	368	GLN
1	R	241	GLN
1	R	259	ASN
1	R	270	HIS
1	R	365	GLN
2	n	215	GLN
2	j	77	ASN
2	k	32	ASN
2	k	77	ASN
2	k	215	GLN
2	o	77	ASN
2	o	215	GLN
2	p	77	ASN
2	q	207	ASN
2	a	77	ASN
2	d	77	ASN
2	g	77	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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.

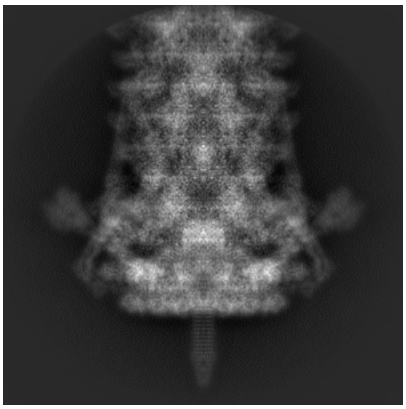
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37152. These allow visual inspection of the internal detail of the map and identification of artifacts.

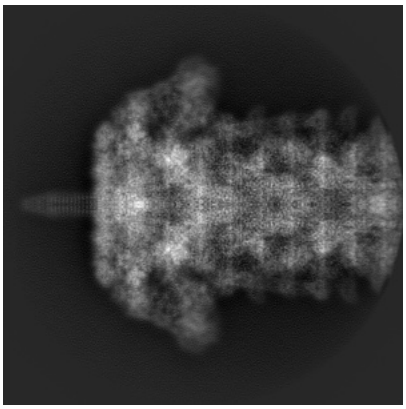
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

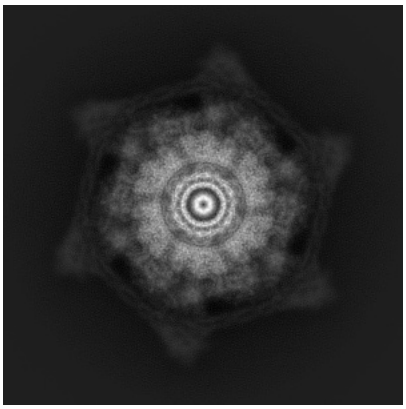
6.1.1 Primary map



X

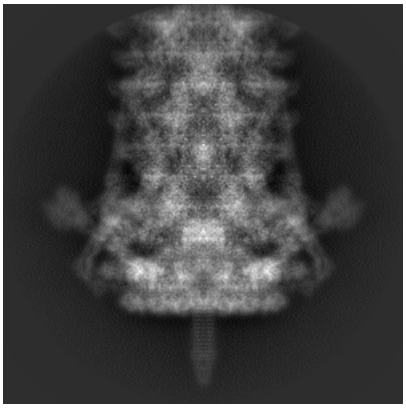


Y

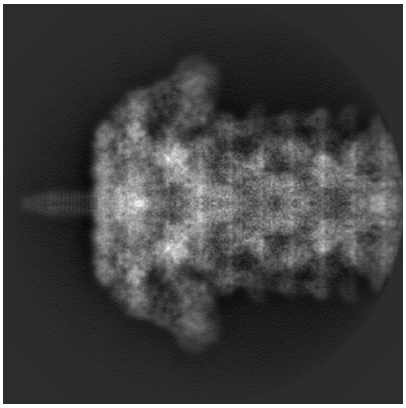


Z

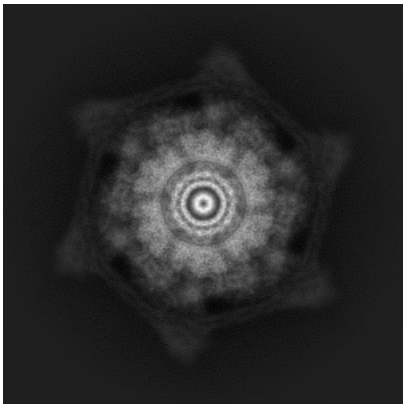
6.1.2 Raw map



X



Y

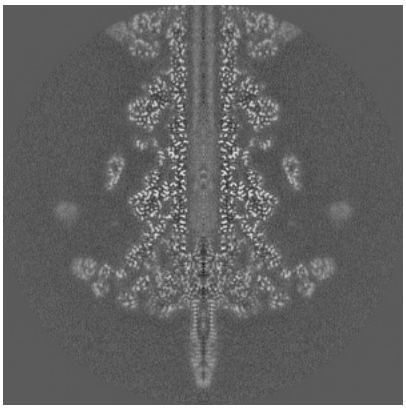


Z

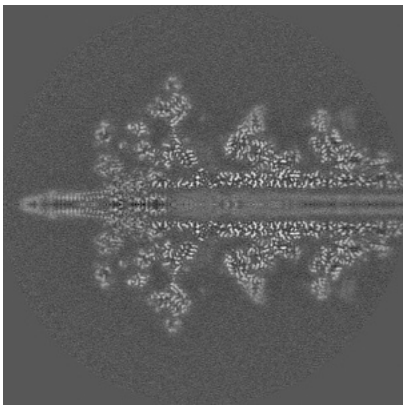
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

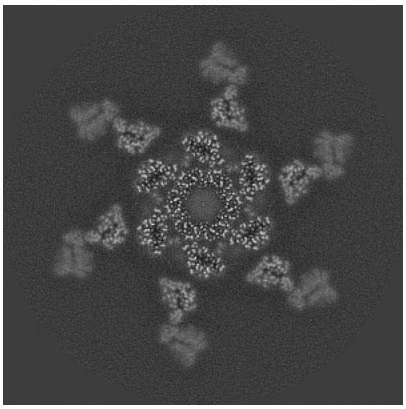
6.2.1 Primary map



X Index: 224

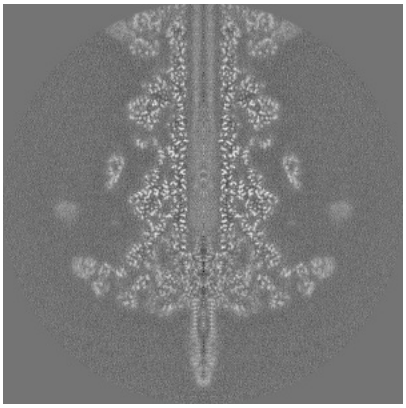


Y Index: 224

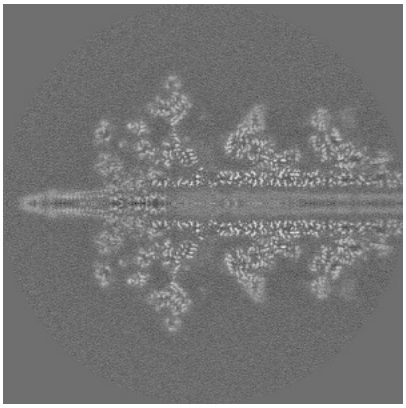


Z Index: 224

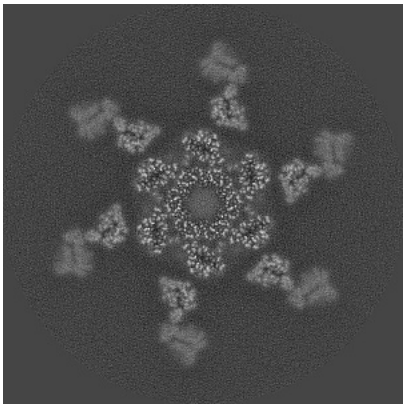
6.2.2 Raw map



X Index: 224



Y Index: 224

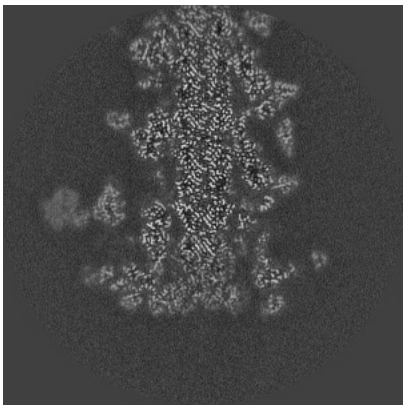


Z Index: 224

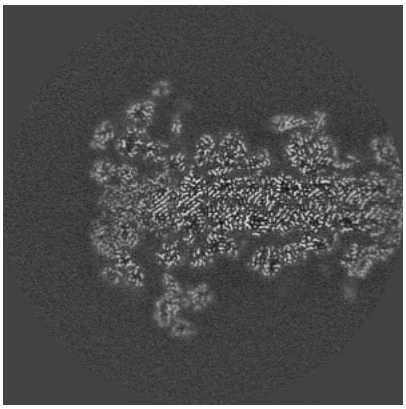
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

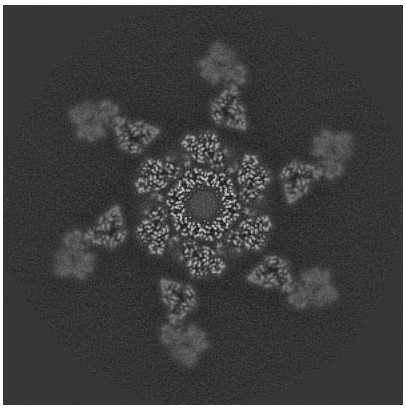
6.3.1 Primary map



X Index: 204

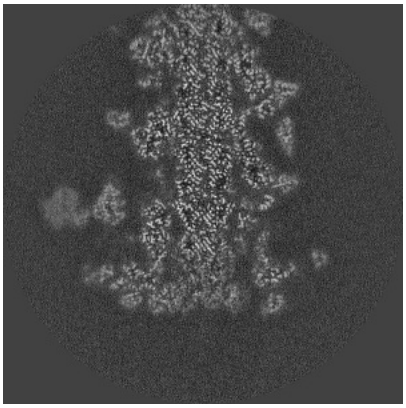


Y Index: 204

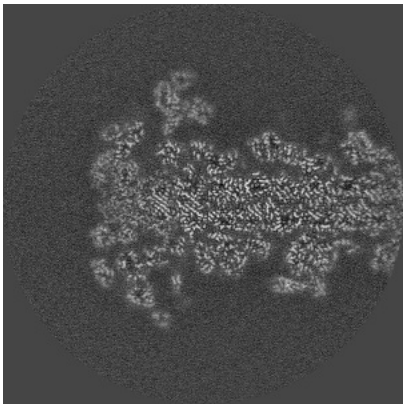


Z Index: 221

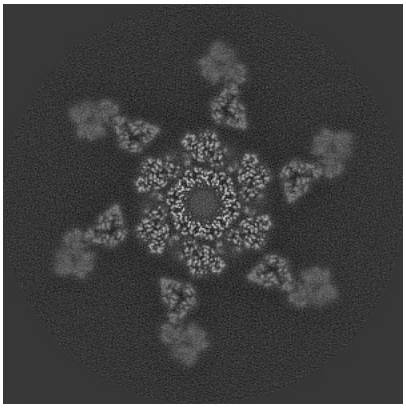
6.3.2 Raw map



X Index: 204



Y Index: 244

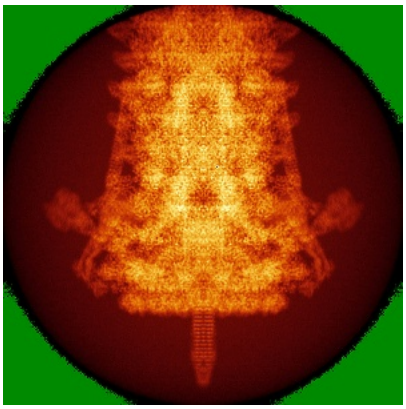


Z Index: 221

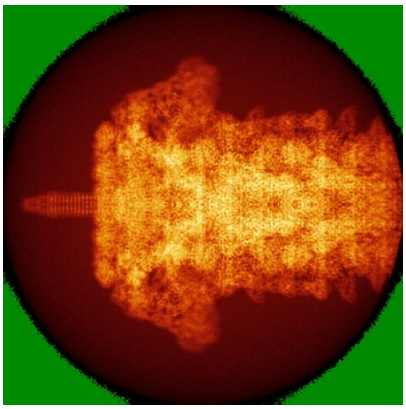
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

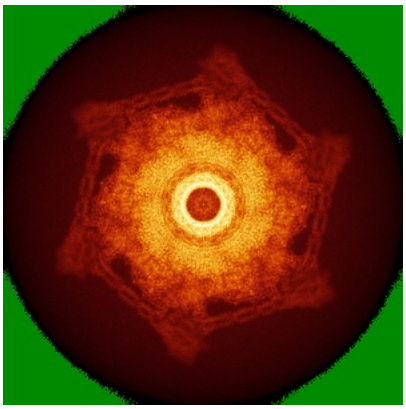
6.4.1 Primary map



X

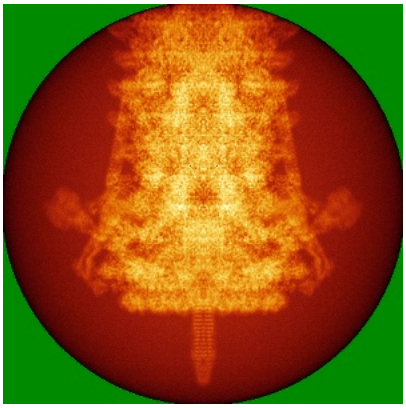


Y

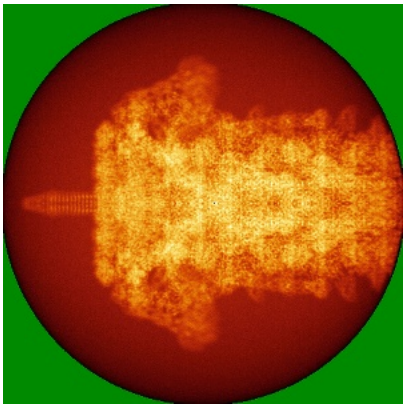


Z

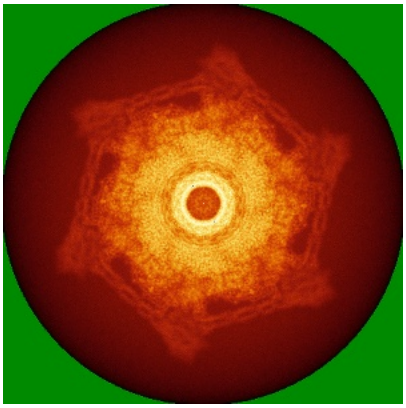
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

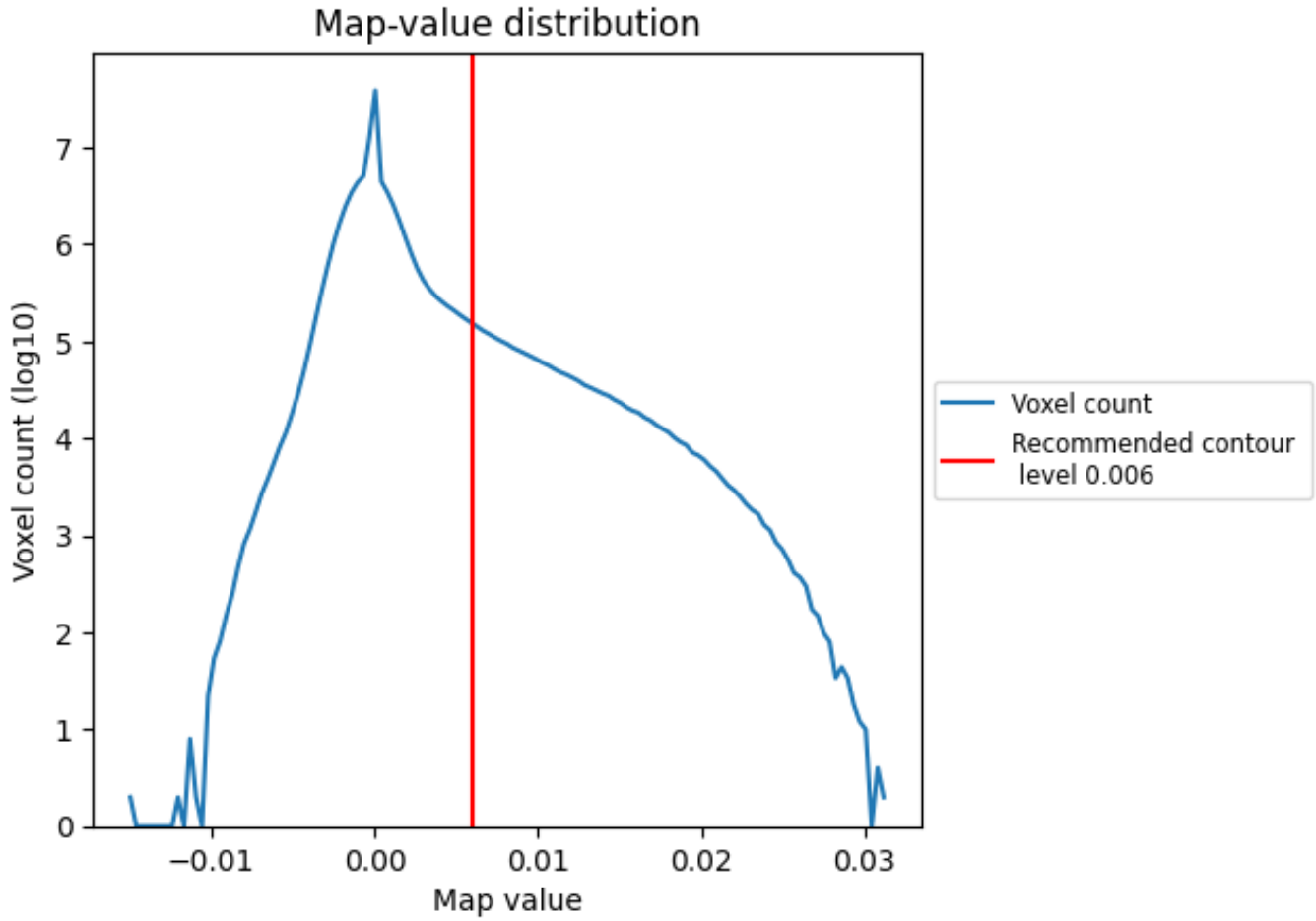
6.6 Mask visualisation (i)

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

7 Map analysis

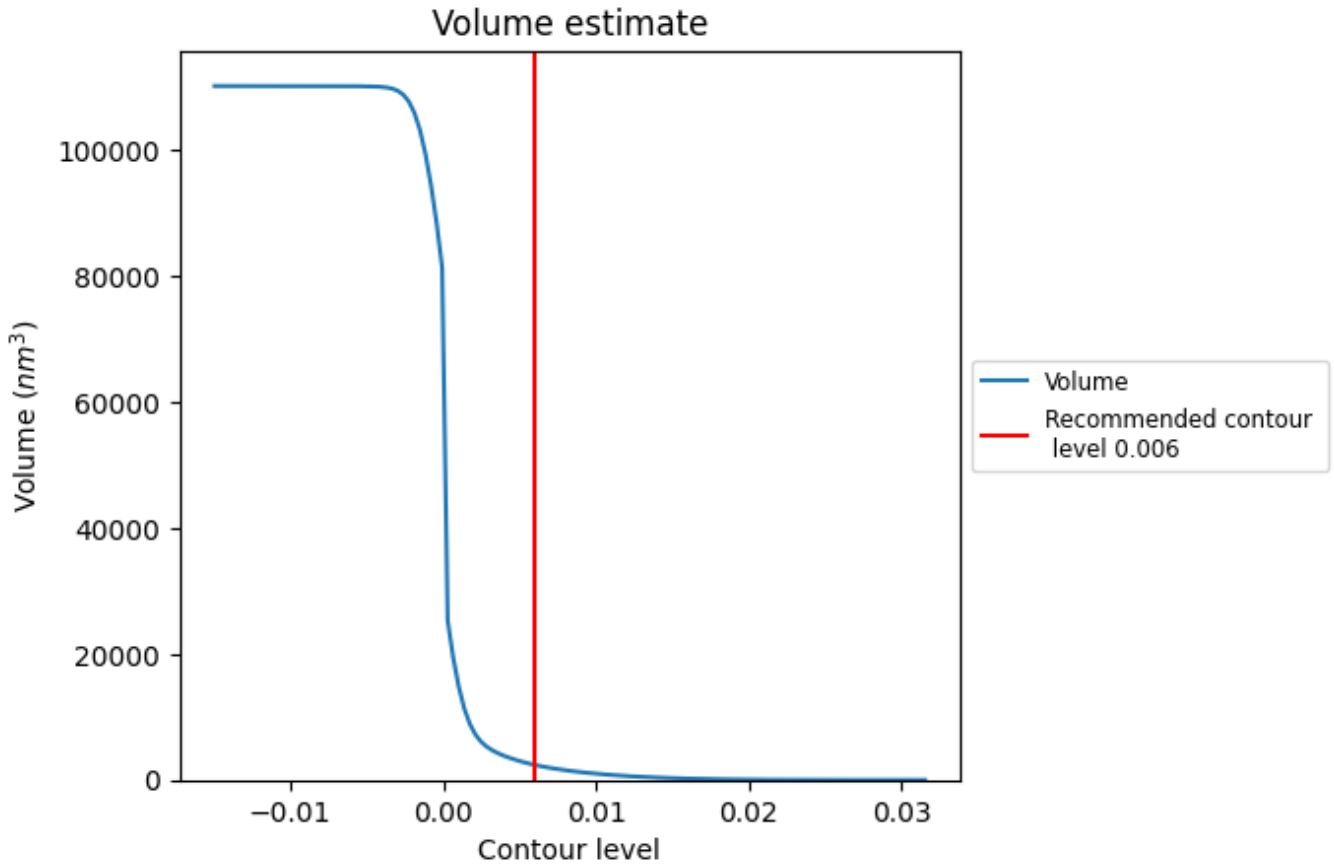
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

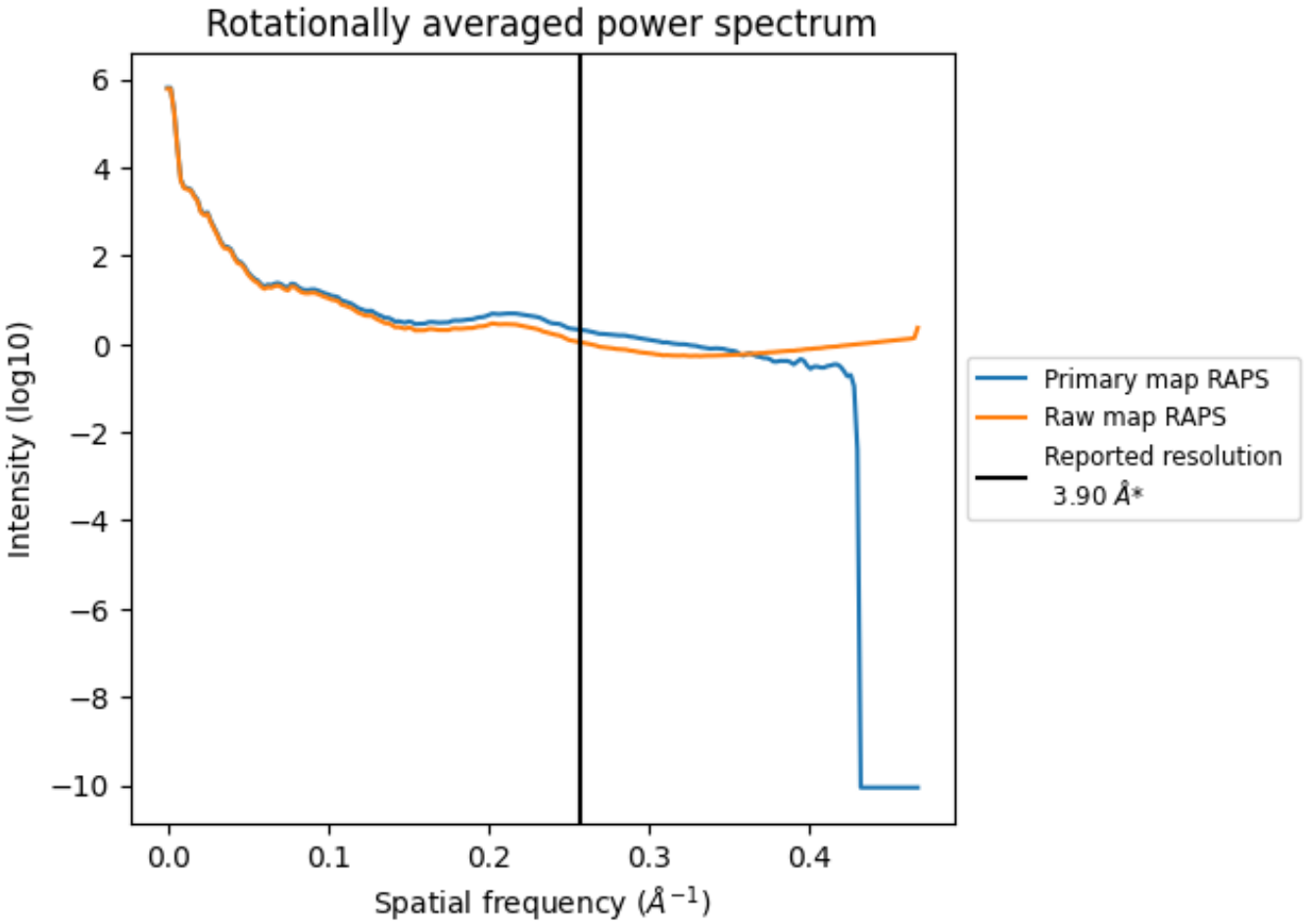
7.2 Volume estimate



The volume at the recommended contour level is 2387 nm^3; this corresponds to an approximate mass of 2157 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

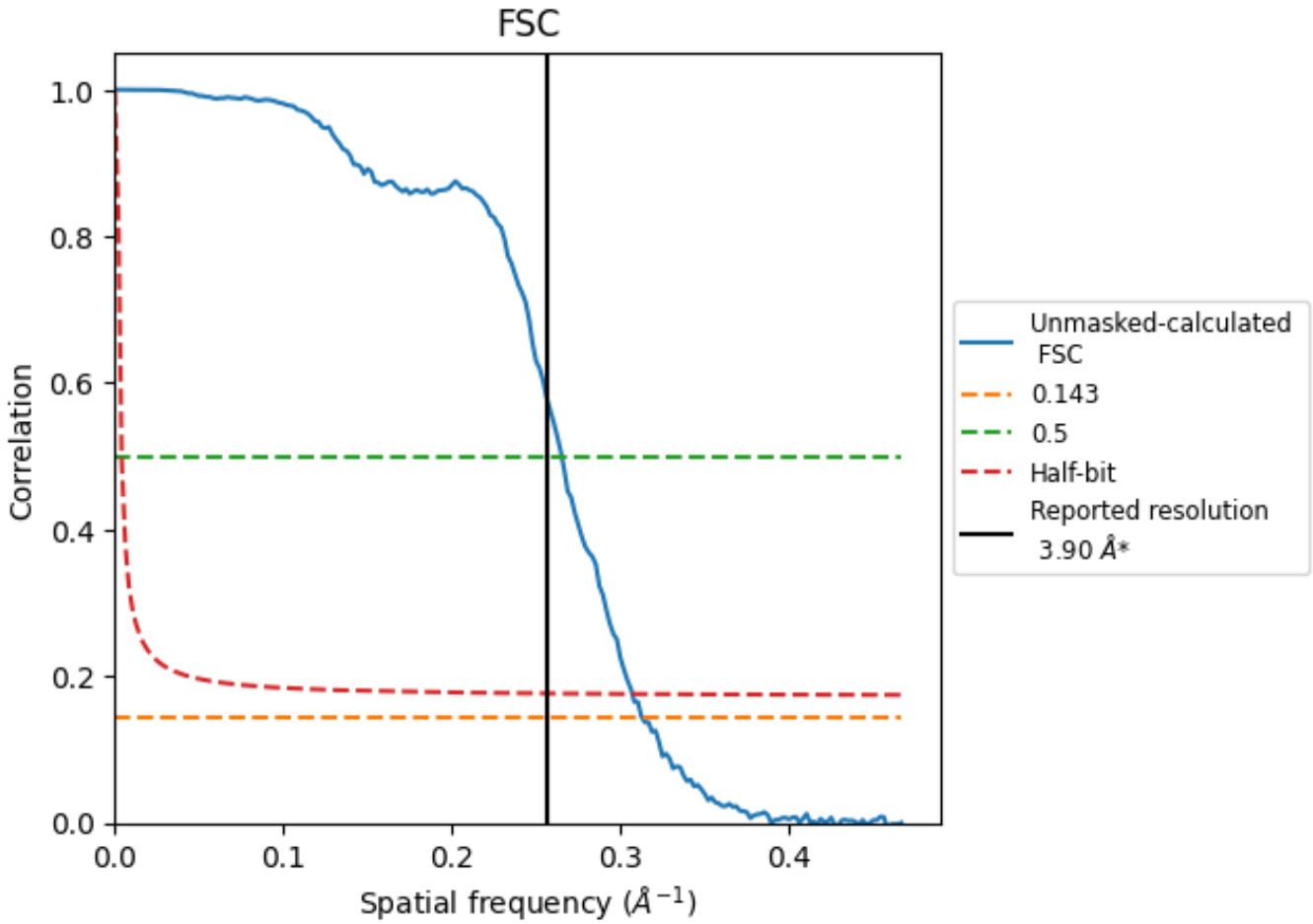


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

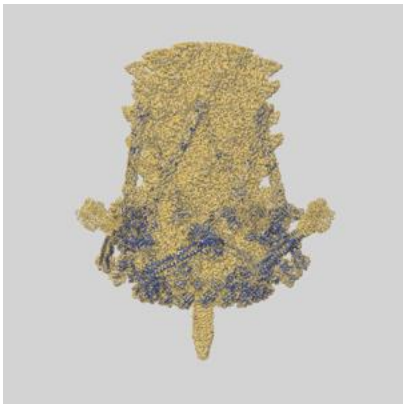
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.77	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 3.9 by more than 10 %

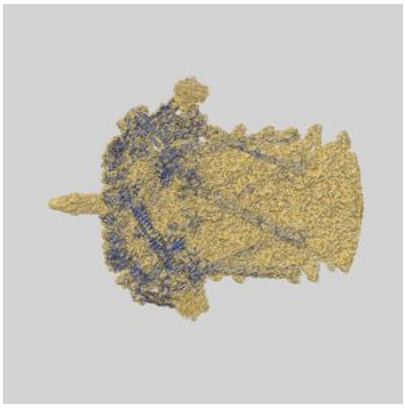
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37152 and PDB model 8KEC. Per-residue inclusion information can be found in section 3 on page 7.

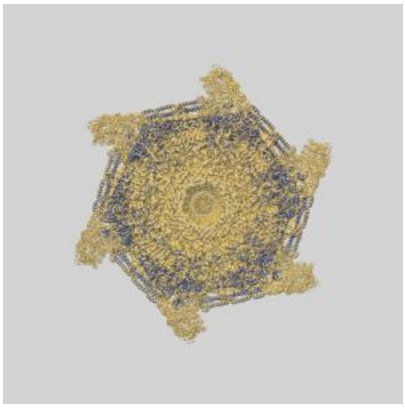
9.1 Map-model overlay



X



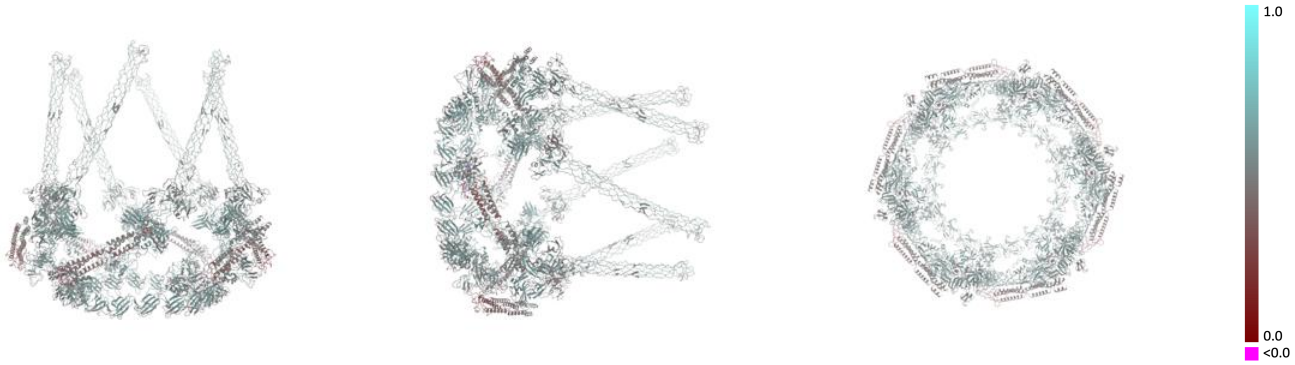
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

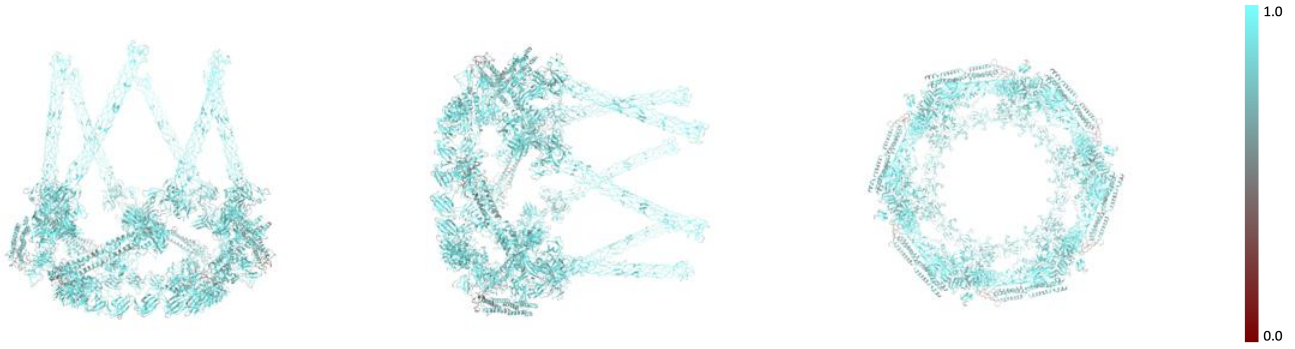
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

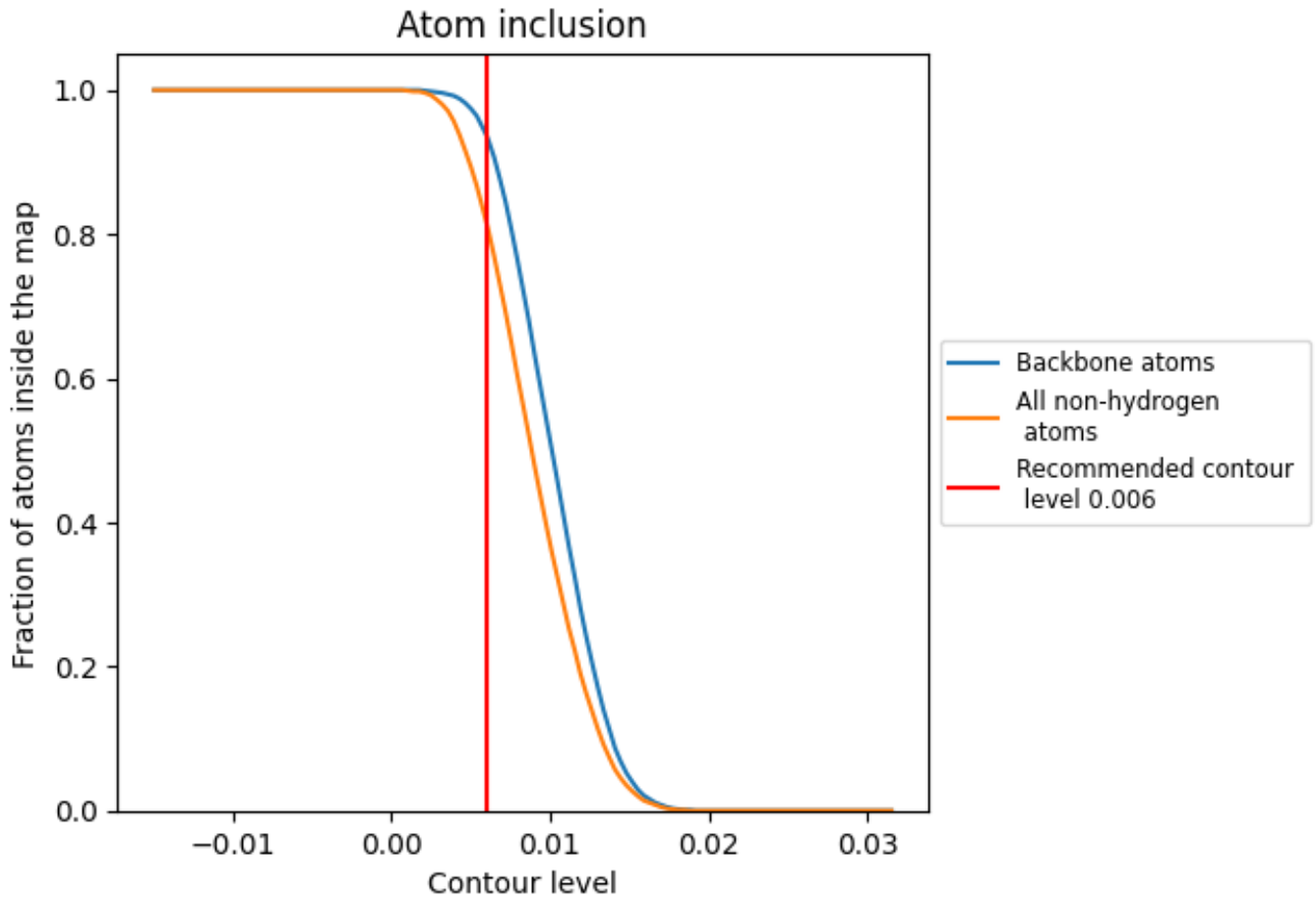
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.5100
A	0.8520	0.5260
B	0.8570	0.5360
C	0.8530	0.5380
D	0.8460	0.5260
E	0.8530	0.5350
F	0.8480	0.5370
G	0.8540	0.5260
H	0.8540	0.5350
I	0.8500	0.5380
J	0.8490	0.5260
K	0.8580	0.5370
L	0.8540	0.5390
M	0.8460	0.5250
N	0.8530	0.5350
O	0.8490	0.5390
P	0.8540	0.5260
Q	0.8550	0.5370
R	0.8500	0.5380
a	0.7620	0.4730
b	0.7540	0.4660
c	0.7950	0.5070
d	0.7670	0.4710
e	0.7510	0.4660
f	0.7930	0.5060
g	0.7650	0.4740
h	0.7450	0.4620
i	0.7940	0.5030
j	0.7680	0.4710
k	0.7470	0.4630
l	0.7900	0.5030
m	0.7630	0.4720
n	0.7240	0.4420
o	0.7870	0.5000
p	0.7620	0.4720

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Chain	Atom inclusion	Q-score
q	0.7490	0.4660
r	0.7930	0.5060