



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 10:39 AM EST

PDB ID : 6UZC
EMDB ID : EMD-20956
Title : Portal vertex structure of bacteriophage T4
Authors : Fang, Q.; Fokine, A.; Rao, V.B.
Deposited on : 2019-11-14
Resolution : 4.50 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:

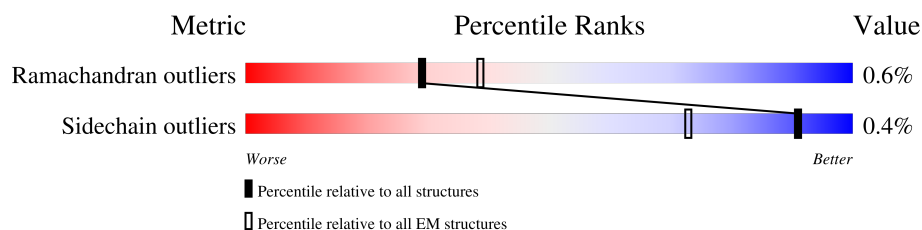
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 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.









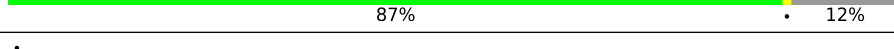
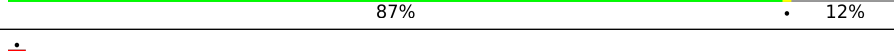
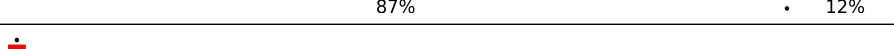
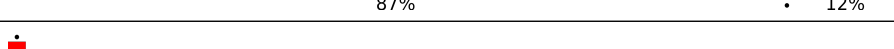
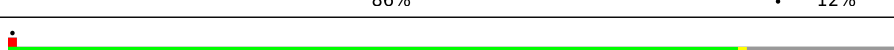

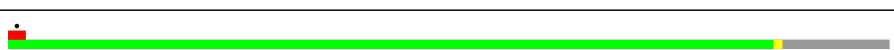

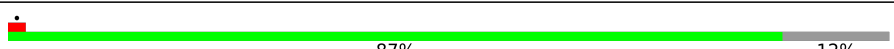





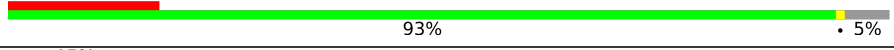
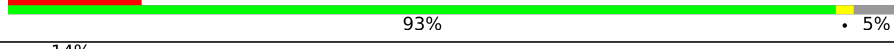
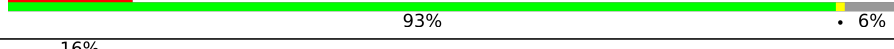
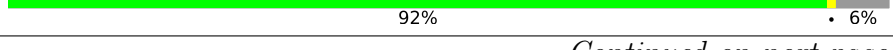

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	521	
1	B	521	
1	C	521	
1	D	521	
1	a	521	
1	b	521	
1	c	521	
1	d	521	
1	e	521	

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Mol	Chain	Length	Quality of chain
1	f	521	
1	g	521	
1	h	521	
1	i	521	
1	j	521	
1	k	521	
1	l	521	
1	m	521	
1	n	521	
1	o	521	
1	p	521	
1	q	521	
1	r	521	
1	s	521	
1	t	521	
1	u	521	
1	v	521	
1	w	521	
1	x	521	
1	y	521	
1	z	521	
2	E	524	
2	F	524	
2	G	524	
2	H	524	

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Mol	Chain	Length	Quality of chain
2	I	524	<div><div>15%</div><div>93%</div><div>6%</div></div>
2	J	524	<div><div>13%</div><div>93%</div><div>6%</div></div>
2	K	524	<div><div>14%</div><div>94%</div><div>5%</div></div>
2	L	524	<div><div>14%</div><div>92%</div><div>6%</div></div>
2	M	524	<div><div>13%</div><div>94%</div><div>5%</div></div>
2	N	524	<div><div>14%</div><div>93%</div><div>6%</div></div>
2	O	524	<div><div>15%</div><div>93%</div><div>6%</div></div>
2	P	524	<div><div>15%</div><div>93%</div><div>5%</div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 150312 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	b	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	c	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	d	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	e	430	Total	C	N	O	S	0	0
			3249	2062	552	620	15		
1	f	456	Total	C	N	O	S	0	0
			3418	2161	584	658	15		
1	g	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	h	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	i	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	j	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	k	430	Total	C	N	O	S	0	0
			3245	2060	552	618	15		
1	l	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	m	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	n	456	Total	C	N	O	S	0	0
			3418	2161	584	658	15		
1	o	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	p	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	q	430	Total	C	N	O	S	0	0
			3245	2060	552	618	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	r	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	s	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	t	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	u	456	Total	C	N	O	S	0	0
			3421	2165	583	658	15		
1	v	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	w	430	Total	C	N	O	S	0	0
			3249	2062	552	620	15		
1	x	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	y	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	z	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	A	456	Total	C	N	O	S	0	0
			3418	2161	584	658	15		
1	B	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	C	430	Total	C	N	O	S	0	0
			3236	2052	550	619	15		
1	D	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

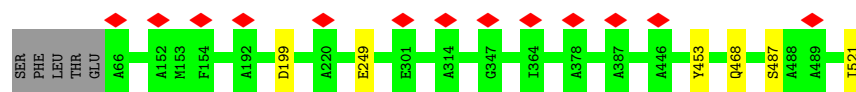
- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	496	Total	C	N	O	S	0	0
			4067	2571	704	770	22		
2	F	496	Total	C	N	O	S	0	0
			4060	2565	704	769	22		
2	G	492	Total	C	N	O	S	0	0
			4018	2538	695	764	21		
2	H	490	Total	C	N	O	S	0	0
			4016	2536	696	763	21		
2	I	492	Total	C	N	O	S	0	0
			4024	2541	698	764	21		
2	J	492	Total	C	N	O	S	0	0
			4024	2541	698	764	21		

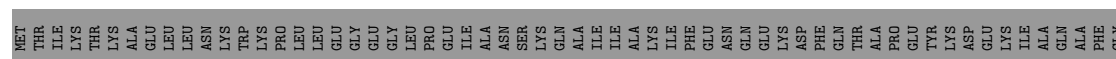
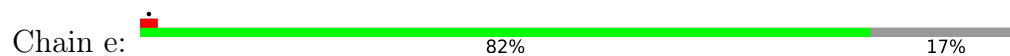
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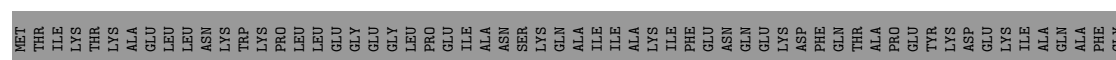
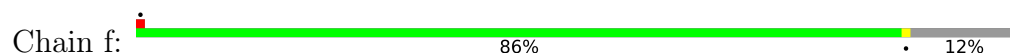
Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	496	Total 4064	C 2570	N 704	O 768	S 22	0	0
2	L	491	Total 4013	C 2533	N 696	O 763	S 21	0	0
2	M	496	Total 4067	C 2571	N 704	O 770	S 22	0	0
2	N	491	Total 4013	C 2533	N 695	O 764	S 21	0	0
2	O	495	Total 4059	C 2566	N 703	O 769	S 21	0	0
2	P	496	Total 4063	C 2568	N 703	O 770	S 22	0	0



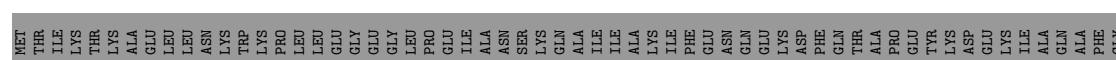
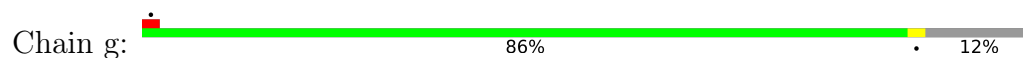
- Molecule 1: Major capsid protein



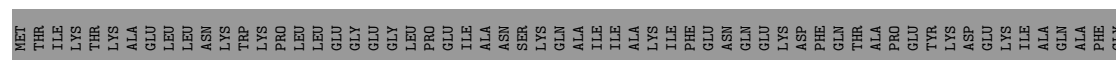
- Molecule 1: Major capsid protein



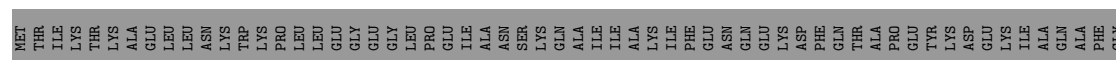
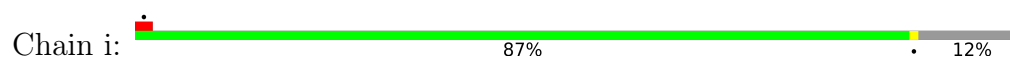
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



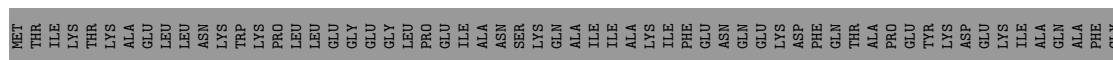
- Molecule 1: Major capsid protein





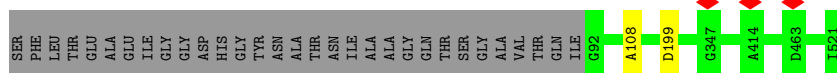
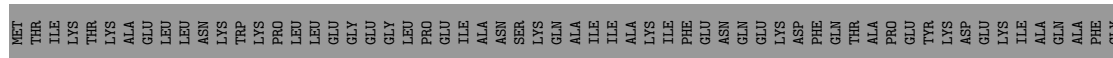
- Molecule 1: Major capsid protein

Chain j: 87% 12%



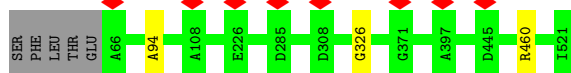
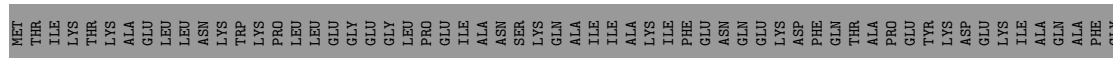
- Molecule 1: Major capsid protein

Chain k: 82% 17%



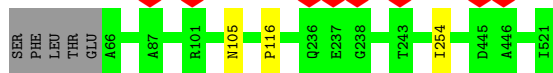
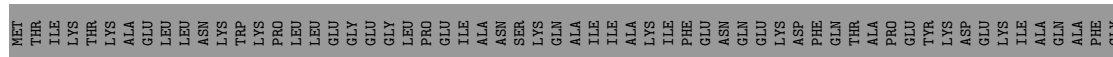
- Molecule 1: Major capsid protein

Chain l: 87% 12%



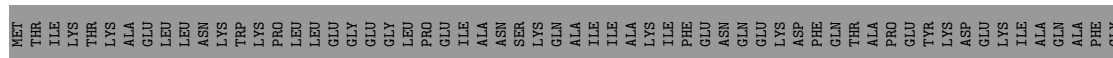
- Molecule 1: Major capsid protein

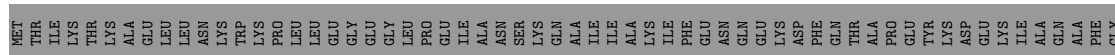
Chain m: 87% 12%

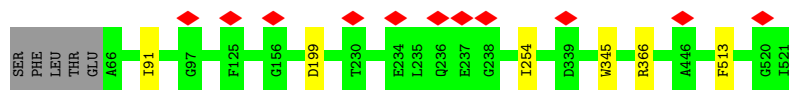


- Molecule 1: Major capsid protein

Chain n: 87% 12%

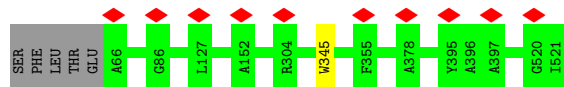
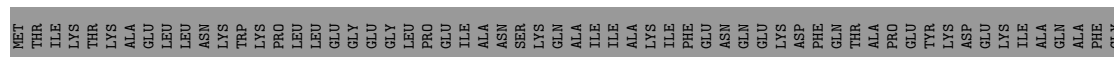






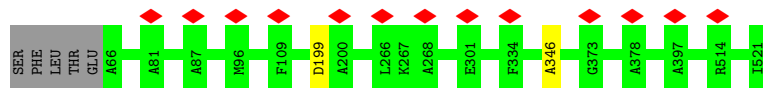
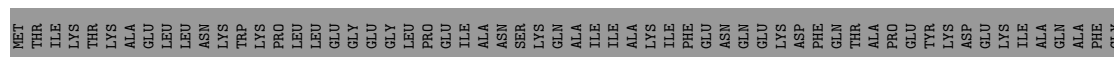
- Molecule 1: Major capsid protein

Chain t: 87% 12%



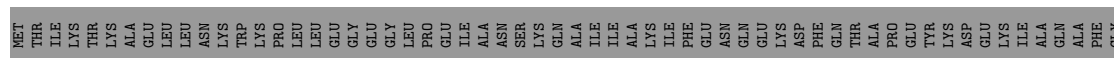
- Molecule 1: Major capsid protein

Chain u: 87% 12%



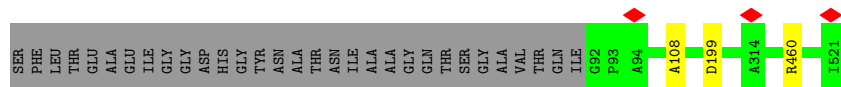
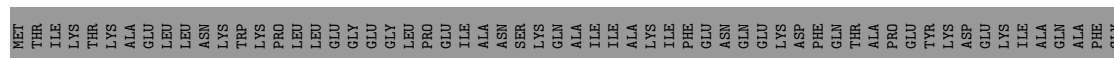
- Molecule 1: Major capsid protein

Chain v: 86% 12%



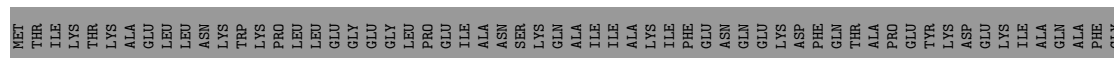
- Molecule 1: Major capsid protein

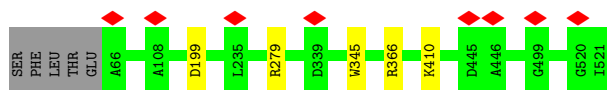
Chain w: 82% 17%



- Molecule 1: Major capsid protein

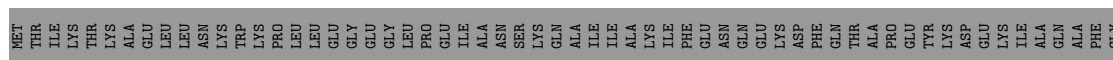
Chain x: 87% 12%





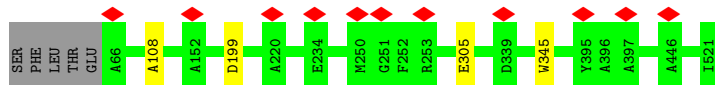
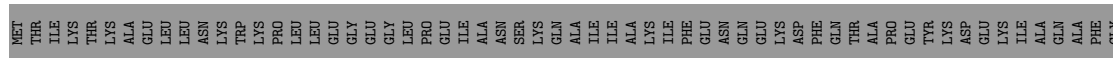
- Molecule 1: Major capsid protein

Chain y: 86% 12%



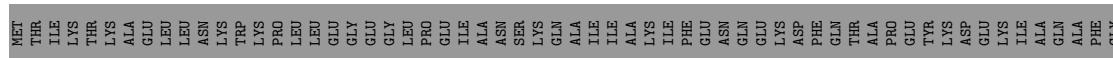
- Molecule 1: Major capsid protein

Chain z: 87% 12%



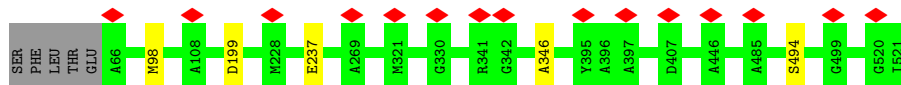
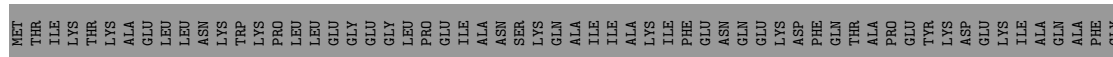
- Molecule 1: Major capsid protein

Chain A: 87% 12%



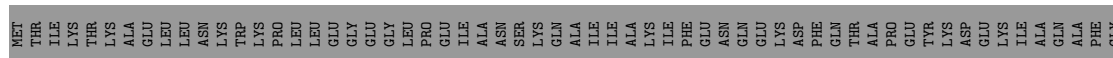
- Molecule 1: Major capsid protein

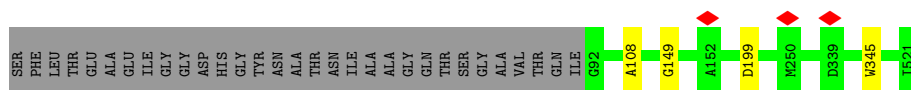
Chain B: 87% 12%



- Molecule 1: Major capsid protein

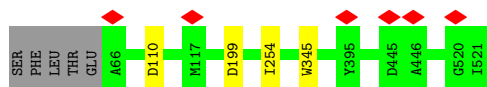
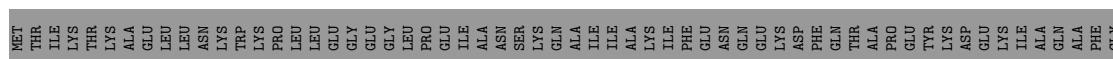
Chain C: 82% 17%





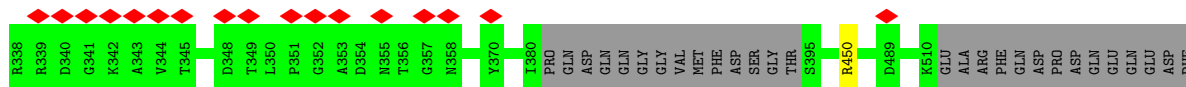
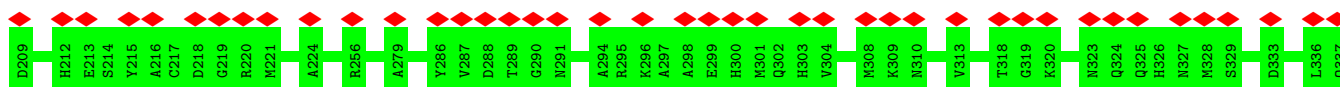
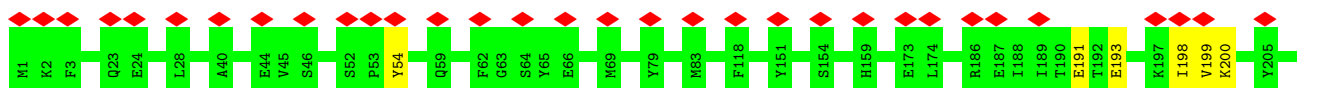
- Molecule 1: Major capsid protein

Chain D: 87% 12%



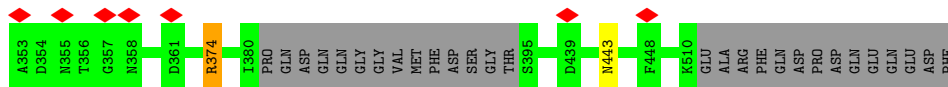
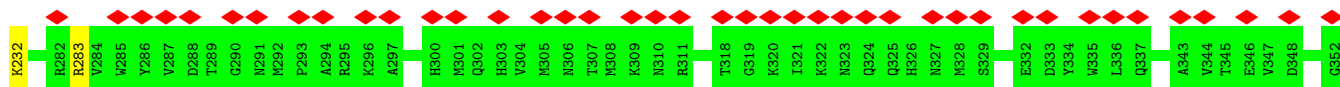
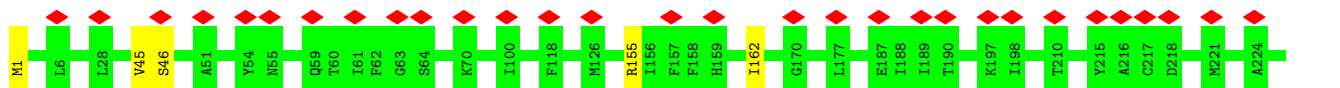
- Molecule 2: Portal protein

Chain E: 17% 93% 5%



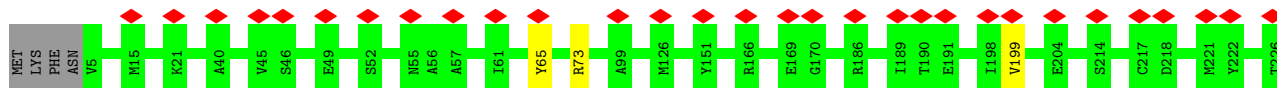
- Molecule 2: Portal protein

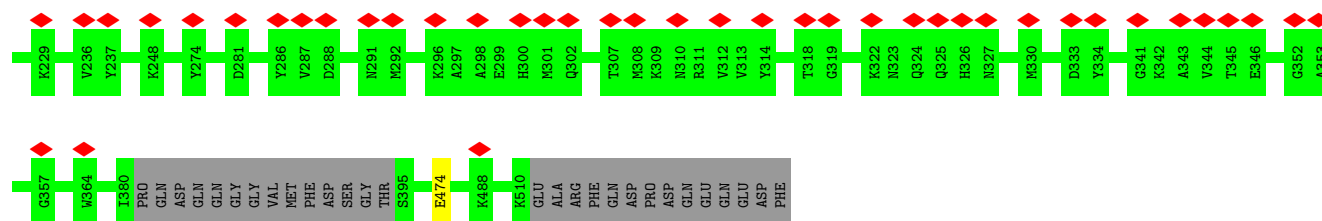
Chain F: 15% 93% 5%



- Molecule 2: Portal protein

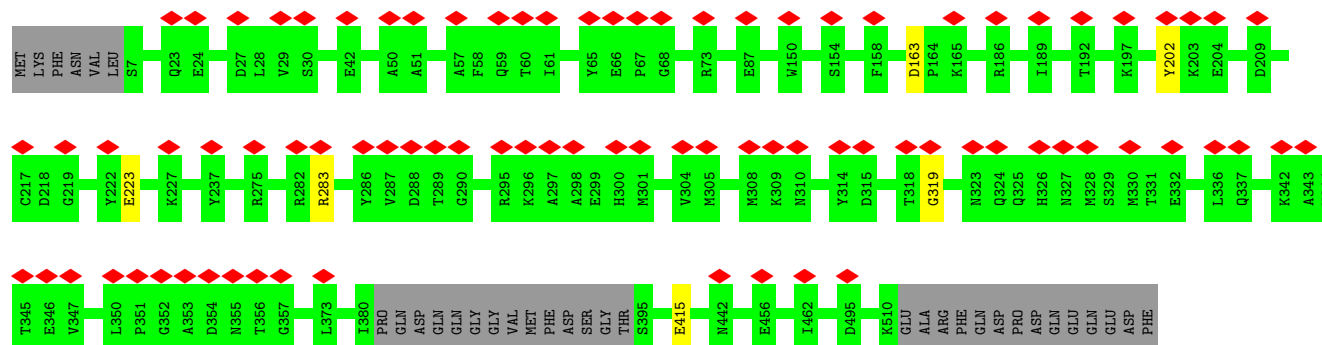
Chain G: 14% 93% 6%





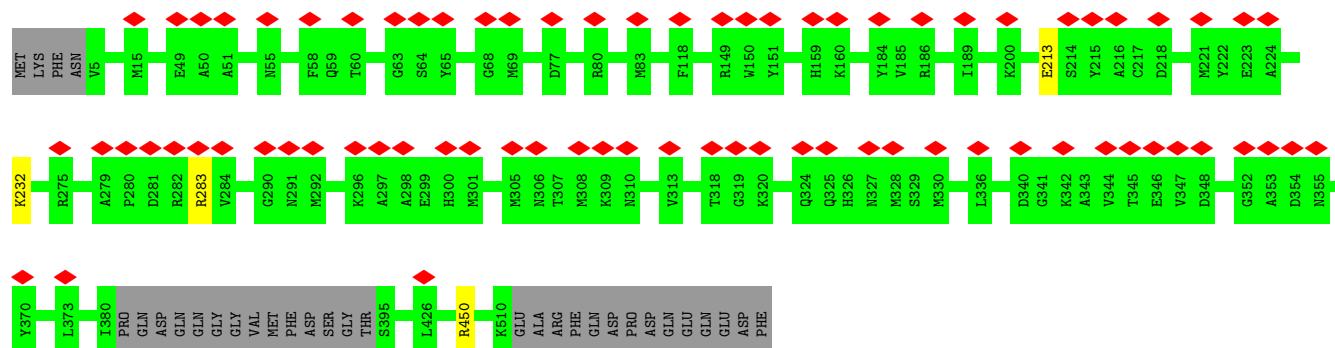
• Molecule 2: Portal protein

Chain H: 16% 92% 6%



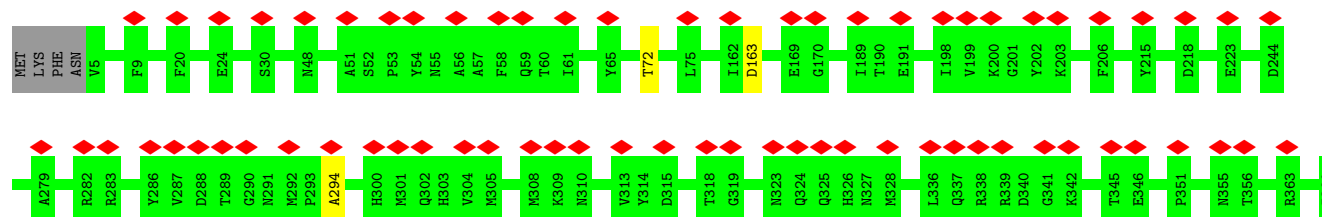
• Molecule 2: Portal protein

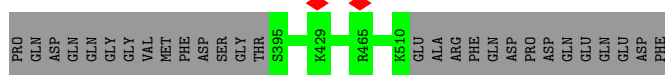
Chain I: 15% 93% 6%



• Molecule 2: Portal protein

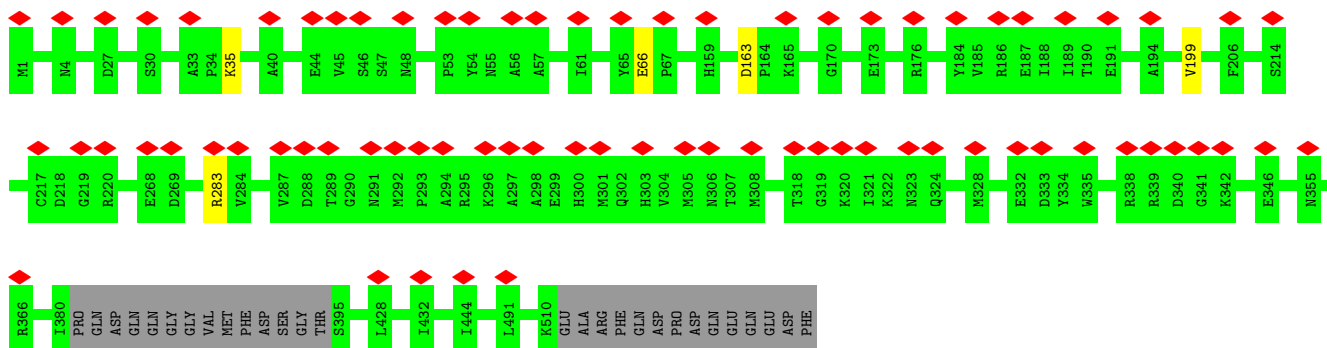
Chain J: 13% 93% 6%





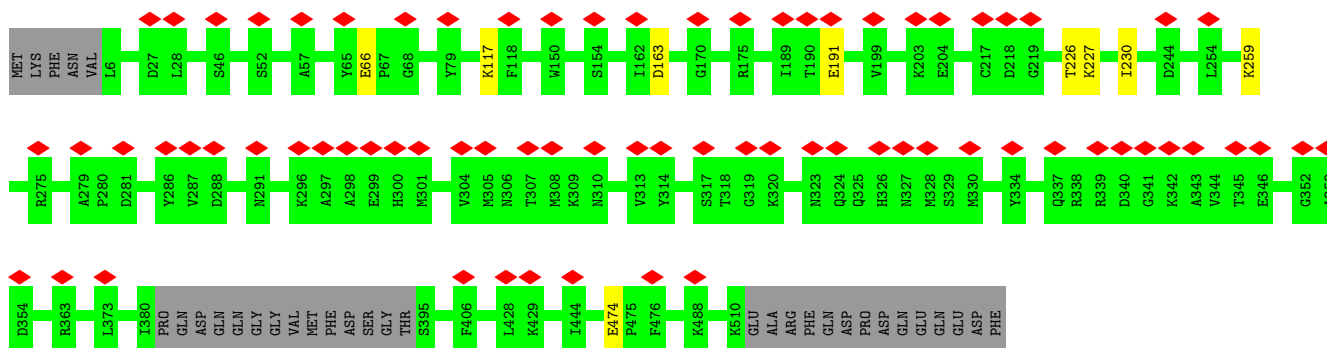
- Molecule 2: Portal protein

Chain K: 14% 94% 5%



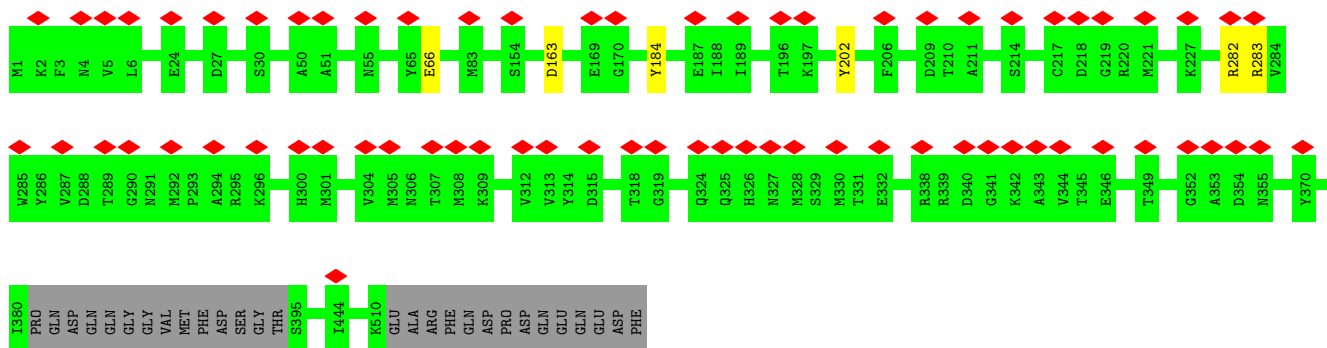
- Molecule 2: Portal protein

Chain L: 14% 92% 6%

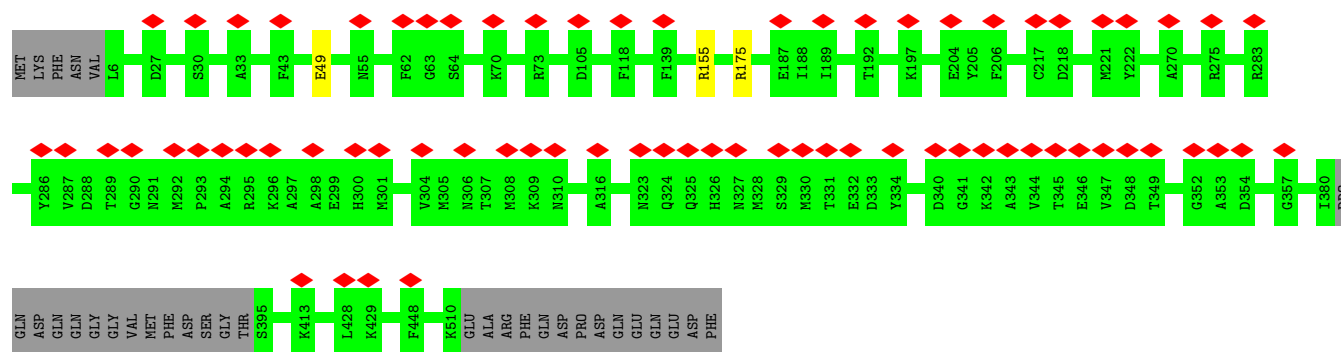
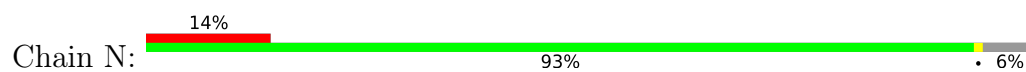


- Molecule 2: Portal protein

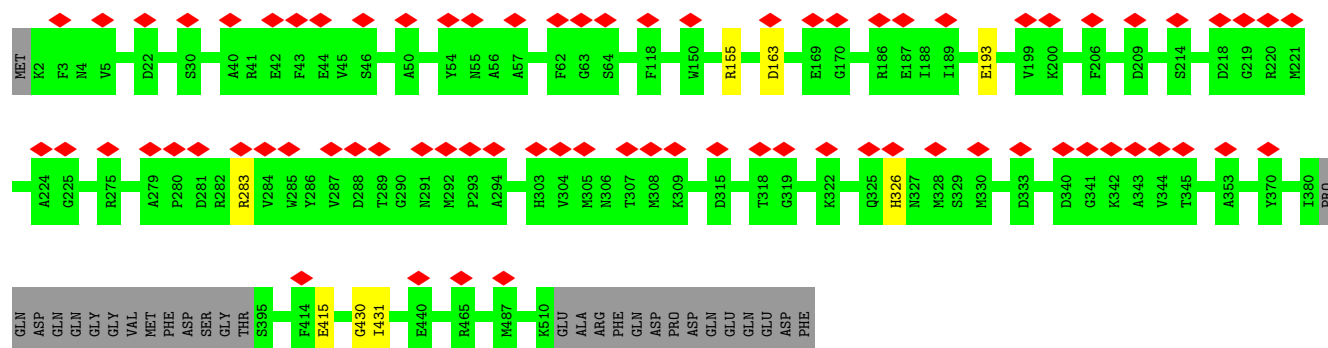
Chain M: 13% 94% 5%



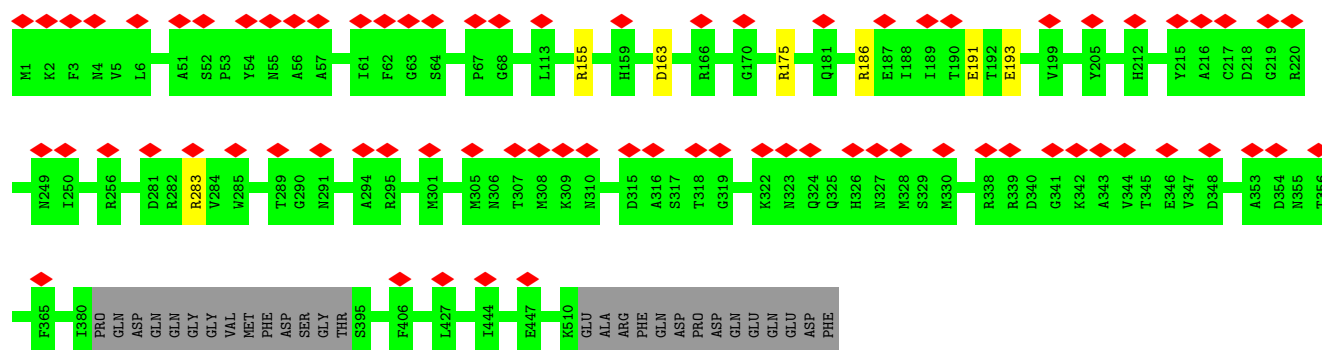
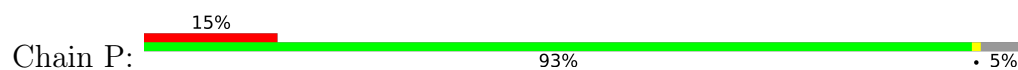
- Molecule 2: Portal protein



• Molecule 2: Portal protein



• Molecule 2: Portal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53608	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 ($e^-/\text{\AA}^2$)	23.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	30.373	Depositor
Minimum map value	-18.707	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.603	Depositor
Recommended contour level	2.5	Depositor
Map size (\AA)	720.0, 720.0, 720.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.44, 1.44, 1.44	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	0.92	0/3485	0.91	0/4720
1	B	0.91	0/3493	0.92	0/4731
1	C	0.96	0/3300	0.92	0/4467
1	D	0.97	0/3493	0.90	0/4731
1	a	0.94	0/3493	0.93	0/4731
1	b	0.92	0/3493	0.95	0/4731
1	c	0.89	0/3493	0.89	0/4731
1	d	0.93	0/3493	0.93	0/4731
1	e	0.93	0/3315	0.91	0/4488
1	f	0.94	0/3485	0.92	0/4720
1	g	0.98	0/3493	0.94	0/4731
1	h	0.90	0/3493	0.92	0/4731
1	i	0.90	0/3493	0.91	0/4731
1	j	0.90	0/3493	0.92	0/4731
1	k	0.92	0/3311	0.92	0/4483
1	l	0.96	0/3493	0.97	0/4731
1	m	0.95	0/3493	0.92	0/4731
1	n	0.92	0/3485	0.90	0/4720
1	o	0.93	0/3493	0.91	0/4731
1	p	0.93	0/3493	0.93	0/4731
1	q	0.94	0/3311	0.93	0/4483
1	r	0.96	0/3493	0.93	0/4731
1	s	0.95	0/3493	0.93	0/4731
1	t	0.88	0/3493	0.90	0/4731
1	u	0.90	0/3489	0.91	0/4726
1	v	0.91	0/3493	0.92	0/4731
1	w	0.99	0/3315	0.90	0/4488
1	x	0.98	0/3493	0.91	0/4731
1	y	0.96	0/3493	0.94	0/4731
1	z	0.91	0/3493	0.92	0/4731
2	E	1.00	0/4147	0.90	0/5588
2	F	0.97	0/4139	0.88	0/5577
2	G	0.99	0/4096	0.87	0/5522
2	H	0.98	0/4095	0.87	0/5519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	I	1.01	0/4102	0.88	0/5529
2	J	1.01	0/4102	0.89	0/5529
2	K	1.01	0/4144	0.91	0/5584
2	L	1.03	0/4091	0.91	1/5515 (0.0%)
2	M	1.00	0/4147	0.86	0/5588
2	N	0.98	0/4090	0.88	0/5513
2	O	0.97	0/4139	0.87	0/5578
2	P	0.99	0/4143	0.90	0/5584
All	All	0.95	0/153284	0.91	1/207272 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	g	0	2
1	p	0	1
2	O	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	227	LYS	C-N-CA	-5.40	108.21	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	O	430	GLY	Peptide
1	g	104	PRO	Peptide
1	g	118	ASN	Peptide
1	p	164	PRO	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	454/521 (87%)	435 (96%)	17 (4%)	2 (0%)	34	72
1	B	454/521 (87%)	434 (96%)	16 (4%)	4 (1%)	17	56
1	C	428/521 (82%)	398 (93%)	26 (6%)	4 (1%)	17	56
1	D	454/521 (87%)	433 (95%)	18 (4%)	3 (1%)	22	62
1	a	454/521 (87%)	419 (92%)	32 (7%)	3 (1%)	22	62
1	b	454/521 (87%)	433 (95%)	20 (4%)	1 (0%)	47	81
1	c	454/521 (87%)	425 (94%)	26 (6%)	3 (1%)	22	62
1	d	454/521 (87%)	426 (94%)	24 (5%)	4 (1%)	17	56
1	e	428/521 (82%)	405 (95%)	21 (5%)	2 (0%)	29	68
1	f	454/521 (87%)	426 (94%)	23 (5%)	5 (1%)	14	52
1	g	454/521 (87%)	426 (94%)	24 (5%)	4 (1%)	17	56
1	h	454/521 (87%)	432 (95%)	21 (5%)	1 (0%)	47	81
1	i	454/521 (87%)	431 (95%)	21 (5%)	2 (0%)	34	72
1	j	454/521 (87%)	432 (95%)	21 (5%)	1 (0%)	47	81
1	k	428/521 (82%)	405 (95%)	21 (5%)	2 (0%)	29	68
1	l	454/521 (87%)	430 (95%)	22 (5%)	2 (0%)	34	72
1	m	454/521 (87%)	425 (94%)	26 (6%)	3 (1%)	22	62
1	n	454/521 (87%)	430 (95%)	23 (5%)	1 (0%)	47	81
1	o	454/521 (87%)	430 (95%)	22 (5%)	2 (0%)	34	72
1	p	454/521 (87%)	430 (95%)	22 (5%)	2 (0%)	34	72
1	q	428/521 (82%)	409 (96%)	16 (4%)	3 (1%)	22	62
1	r	454/521 (87%)	432 (95%)	20 (4%)	2 (0%)	34	72
1	s	454/521 (87%)	425 (94%)	25 (6%)	4 (1%)	17	56
1	t	454/521 (87%)	432 (95%)	21 (5%)	1 (0%)	47	81
1	u	454/521 (87%)	433 (95%)	19 (4%)	2 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	454/521 (87%)	428 (94%)	20 (4%)	6 (1%)	12	48
1	w	428/521 (82%)	409 (96%)	17 (4%)	2 (0%)	29	68
1	x	454/521 (87%)	435 (96%)	17 (4%)	2 (0%)	34	72
1	y	454/521 (87%)	425 (94%)	24 (5%)	5 (1%)	14	52
1	z	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	22	62
2	E	492/524 (94%)	460 (94%)	28 (6%)	4 (1%)	19	60
2	F	492/524 (94%)	468 (95%)	21 (4%)	3 (1%)	25	65
2	G	488/524 (93%)	467 (96%)	19 (4%)	2 (0%)	34	72
2	H	486/524 (93%)	461 (95%)	21 (4%)	4 (1%)	19	60
2	I	488/524 (93%)	454 (93%)	33 (7%)	1 (0%)	47	81
2	J	488/524 (93%)	463 (95%)	23 (5%)	2 (0%)	34	72
2	K	492/524 (94%)	459 (93%)	29 (6%)	4 (1%)	19	60
2	L	487/524 (93%)	448 (92%)	33 (7%)	6 (1%)	13	50
2	M	492/524 (94%)	463 (94%)	26 (5%)	3 (1%)	25	65
2	N	487/524 (93%)	461 (95%)	26 (5%)	0	100	100
2	O	491/524 (94%)	460 (94%)	27 (6%)	4 (1%)	19	60
2	P	492/524 (94%)	459 (93%)	31 (6%)	2 (0%)	34	72
All	All	19365/21918 (88%)	18288 (94%)	961 (5%)	116 (1%)	29	65

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	346	ALA
1	f	345	TRP
1	g	345	TRP
1	o	346	ALA
1	s	345	TRP
1	u	346	ALA
1	z	345	TRP
1	A	346	ALA
2	E	199	VAL
2	F	443	ASN
2	I	232	LYS
2	J	294	ALA
2	K	35	LYS
2	K	199	VAL

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Mol	Chain	Res	Type
2	L	226	THR
2	O	163	ASP
2	O	431	ILE
1	a	199	ASP
1	a	254	ILE
1	b	345	TRP
1	f	346	ALA
1	g	254	ILE
1	h	345	TRP
1	j	199	ASP
1	m	254	ILE
1	q	254	ILE
1	q	345	TRP
1	r	345	TRP
1	s	91	ILE
1	s	254	ILE
1	x	345	TRP
1	y	254	ILE
1	y	345	TRP
1	A	199	ASP
1	B	237	GLU
1	B	346	ALA
1	B	494	SER
1	C	149	GLY
1	D	254	ILE
1	D	345	TRP
2	F	374	ARG
2	H	202	TYR
2	H	319	GLY
2	K	163	ASP
2	L	66	GLU
2	O	326	HIS
1	a	116	PRO
1	c	487	SER
1	d	199	ASP
1	d	487	SER
1	f	199	ASP
1	f	494	SER
1	i	199	ASP
1	l	94	ALA
1	l	326	GLY
1	m	105	ASN

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Mol	Chain	Res	Type
1	o	115	GLN
1	p	199	ASP
1	q	199	ASP
1	s	199	ASP
1	t	345	TRP
1	u	199	ASP
1	v	199	ASP
1	v	494	SER
1	w	199	ASP
1	x	199	ASP
1	y	199	ASP
1	z	199	ASP
1	C	108	ALA
1	C	199	ASP
2	E	54	TYR
2	H	415	GLU
2	K	66	GLU
2	M	202	TYR
2	O	415	GLU
2	P	163	ASP
1	c	199	ASP
1	f	404	PHE
1	g	199	ASP
1	k	108	ALA
1	k	199	ASP
1	m	116	PRO
1	n	345	TRP
1	v	94	ALA
1	v	108	ALA
1	w	108	ALA
1	y	108	ALA
1	y	501	PRO
1	B	199	ASP
1	D	199	ASP
2	G	199	VAL
2	L	474	GLU
2	M	163	ASP
1	d	453	TYR
1	d	468	GLN
1	e	199	ASP
1	e	433	TYR
1	g	108	ALA

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Mol	Chain	Res	Type
1	p	494	SER
1	v	493	ALA
1	z	108	ALA
2	E	200	LYS
2	L	230	ILE
2	L	259	LYS
2	M	66	GLU
2	P	155	ARG
1	i	345	TRP
1	r	453	TYR
1	v	237	GLU
1	C	345	TRP
2	F	46	SER
2	G	474	GLU
2	L	163	ASP
2	E	198	ILE
2	J	163	ASP
2	H	163	ASP

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	344/400 (86%)	344 (100%)	0	100	100
1	B	345/400 (86%)	344 (100%)	1 (0%)	92	95
1	C	327/400 (82%)	327 (100%)	0	100	100
1	D	345/400 (86%)	344 (100%)	1 (0%)	92	95
1	a	345/400 (86%)	344 (100%)	1 (0%)	92	95
1	b	345/400 (86%)	345 (100%)	0	100	100
1	c	345/400 (86%)	345 (100%)	0	100	100
1	d	345/400 (86%)	343 (99%)	2 (1%)	86	92
1	e	329/400 (82%)	329 (100%)	0	100	100
1	f	344/400 (86%)	341 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	345/400 (86%)	342 (99%)	3 (1%)	78	87
1	h	345/400 (86%)	345 (100%)	0	100	100
1	i	345/400 (86%)	344 (100%)	1 (0%)	92	95
1	j	345/400 (86%)	344 (100%)	1 (0%)	92	95
1	k	328/400 (82%)	328 (100%)	0	100	100
1	l	345/400 (86%)	344 (100%)	1 (0%)	92	95
1	m	345/400 (86%)	345 (100%)	0	100	100
1	n	344/400 (86%)	342 (99%)	2 (1%)	86	92
1	o	345/400 (86%)	343 (99%)	2 (1%)	86	92
1	p	345/400 (86%)	342 (99%)	3 (1%)	78	87
1	q	328/400 (82%)	327 (100%)	1 (0%)	92	95
1	r	345/400 (86%)	343 (99%)	2 (1%)	86	92
1	s	345/400 (86%)	343 (99%)	2 (1%)	86	92
1	t	345/400 (86%)	345 (100%)	0	100	100
1	u	344/400 (86%)	344 (100%)	0	100	100
1	v	345/400 (86%)	343 (99%)	2 (1%)	86	92
1	w	329/400 (82%)	328 (100%)	1 (0%)	92	95
1	x	345/400 (86%)	342 (99%)	3 (1%)	78	87
1	y	345/400 (86%)	344 (100%)	1 (0%)	92	95
1	z	345/400 (86%)	344 (100%)	1 (0%)	92	95
2	E	441/465 (95%)	438 (99%)	3 (1%)	84	90
2	F	440/465 (95%)	433 (98%)	7 (2%)	62	79
2	G	435/465 (94%)	433 (100%)	2 (0%)	88	93
2	H	435/465 (94%)	433 (100%)	2 (0%)	88	93
2	I	436/465 (94%)	433 (99%)	3 (1%)	84	90
2	J	436/465 (94%)	435 (100%)	1 (0%)	93	96
2	K	440/465 (95%)	439 (100%)	1 (0%)	93	96
2	L	434/465 (93%)	432 (100%)	2 (0%)	88	93
2	M	441/465 (95%)	438 (99%)	3 (1%)	84	90
2	N	434/465 (93%)	431 (99%)	3 (1%)	84	90
2	O	440/465 (95%)	437 (99%)	3 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	440/465 (95%)	435 (99%)	5 (1%)	73	85
All	All	15514/17580 (88%)	15445 (100%)	69 (0%)	91	94

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	471	MET
1	d	249	GLU
1	d	521	ILE
1	f	345	TRP
1	f	363	GLU
1	f	410	LYS
1	g	253	ARG
1	g	482	ASN
1	g	497	GLN
1	i	449	TYR
1	j	249	GLU
1	l	460	ARG
1	n	250	MET
1	n	438	TYR
1	o	128	ARG
1	o	305	GLU
1	p	249	GLU
1	p	312	TYR
1	p	513	PHE
1	q	410	LYS
1	r	253	ARG
1	r	420	LYS
1	s	366	ARG
1	s	513	PHE
1	v	279	ARG
1	v	312	TYR
1	w	460	ARG
1	x	279	ARG
1	x	366	ARG
1	x	410	LYS
1	y	482	ASN
1	z	305	GLU
1	B	98	MET
1	D	110	ASP
2	E	191	GLU
2	E	193	GLU

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Mol	Chain	Res	Type
2	E	450	ARG
2	F	1	MET
2	F	45	VAL
2	F	155	ARG
2	F	162	ILE
2	F	232	LYS
2	F	283	ARG
2	F	374	ARG
2	G	65	TYR
2	G	73	ARG
2	H	223	GLU
2	H	283	ARG
2	I	213	GLU
2	I	283	ARG
2	I	450	ARG
2	J	72	THR
2	K	283	ARG
2	L	117	LYS
2	L	191	GLU
2	M	184	TYR
2	M	282	ARG
2	M	283	ARG
2	N	49	GLU
2	N	155	ARG
2	N	175	ARG
2	O	155	ARG
2	O	193	GLU
2	O	283	ARG
2	P	175	ARG
2	P	186	ARG
2	P	191	GLU
2	P	193	GLU
2	P	283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	240	ASN
1	c	265	GLN
1	d	72	HIS
1	e	311	ASN
1	e	398	GLN

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Mol	Chain	Res	Type
1	n	115	GLN
1	r	72	HIS
1	r	482	ASN
1	s	303	ASN
1	z	398	GLN
1	A	311	ASN
1	C	311	ASN
1	D	157	GLN
1	D	257	GLN
2	H	327	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

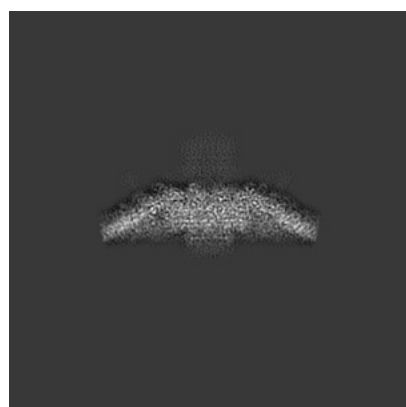
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20956. These allow visual inspection of the internal detail of the map and identification of artifacts.

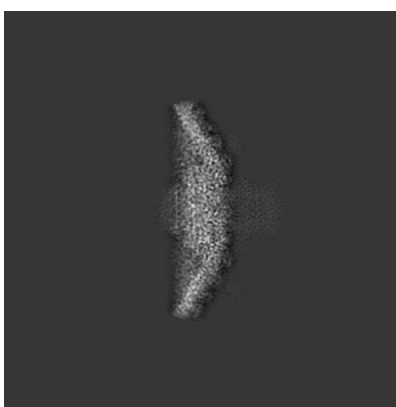
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

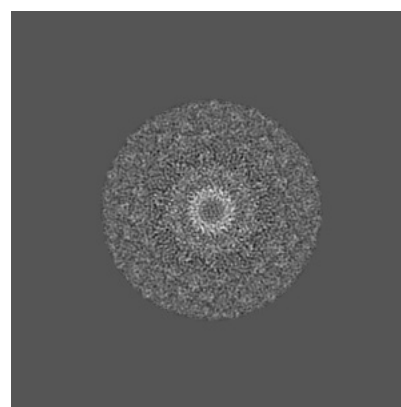
6.1.1 Primary map



X



Y

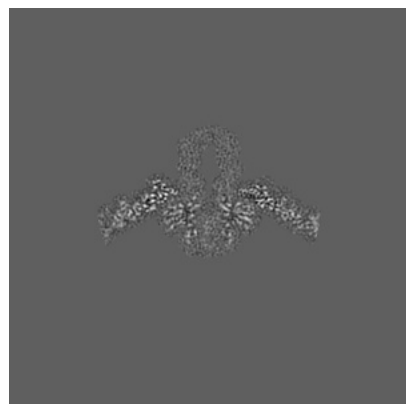


Z

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

6.2 Central slices [i](#)

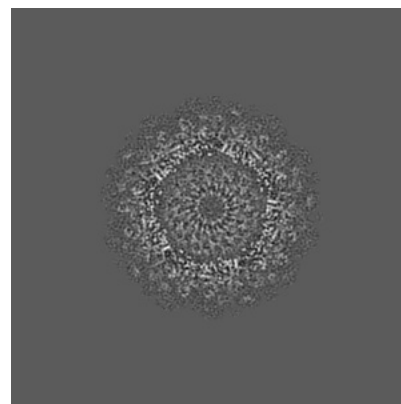
6.2.1 Primary map



X Index: 250



Y Index: 250

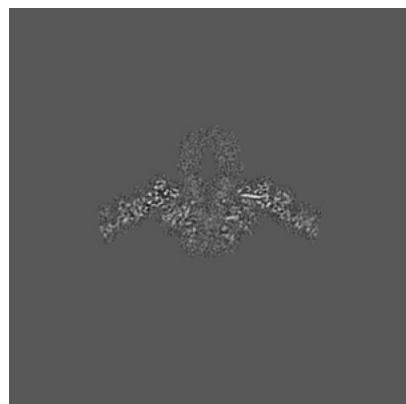


Z Index: 250

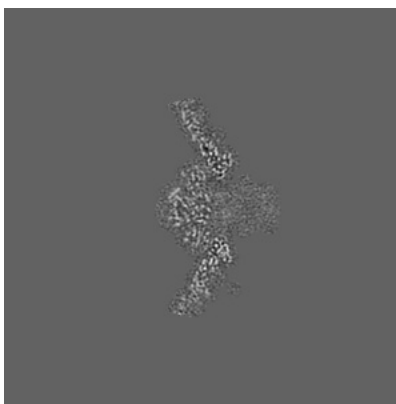
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

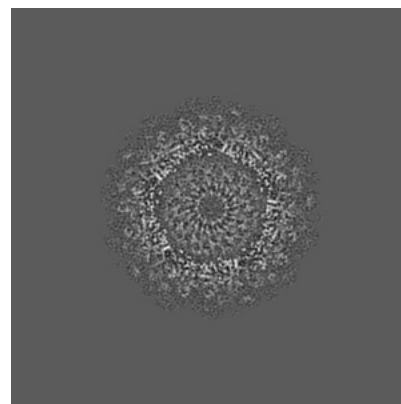
6.3.1 Primary map



X Index: 246



Y Index: 228



Z Index: 250

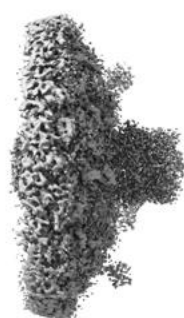
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

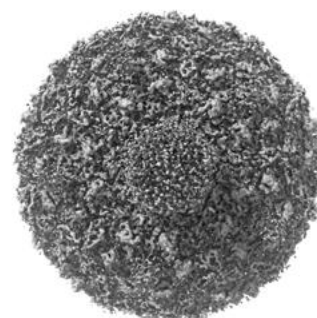
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

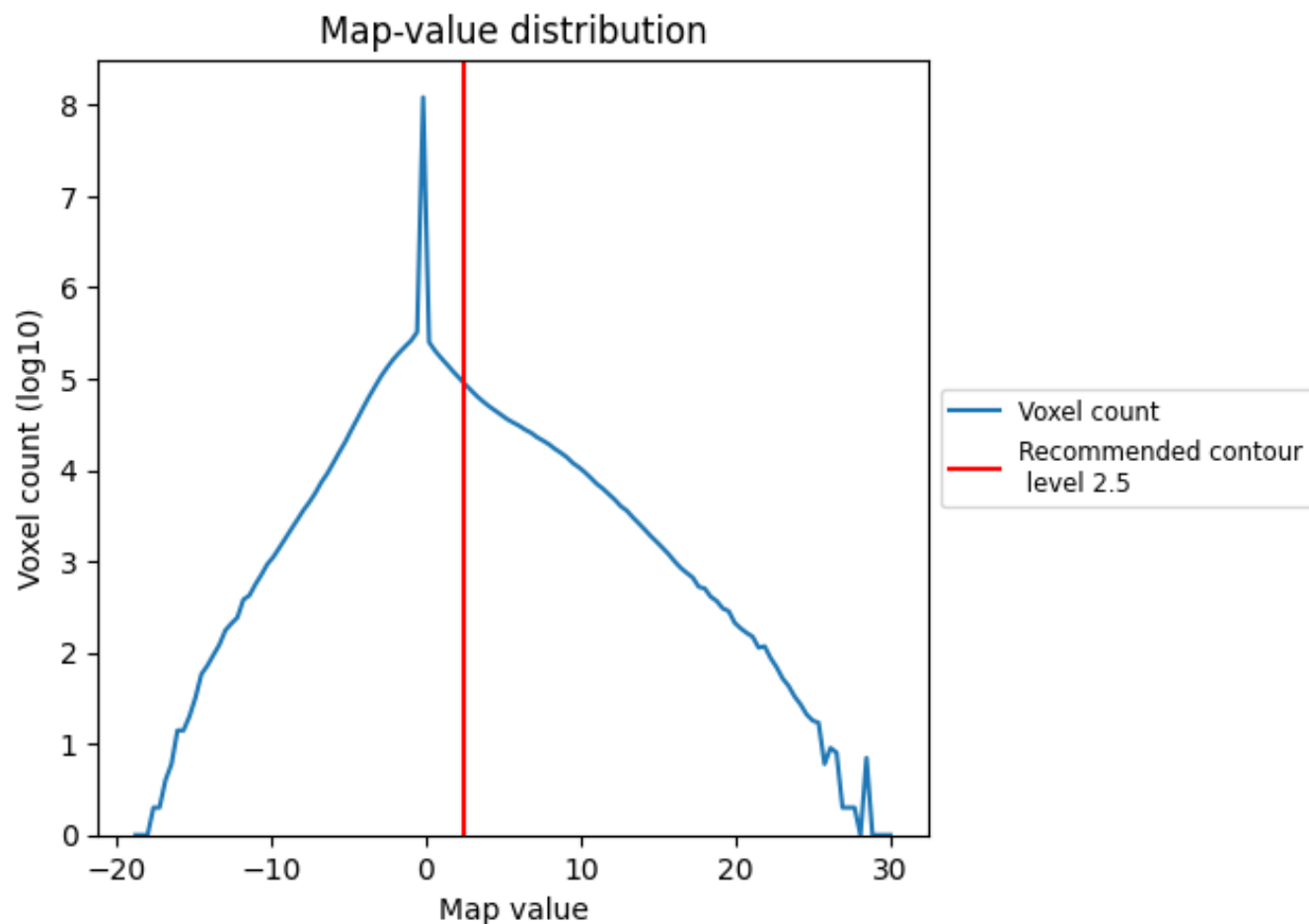
6.5 Mask visualisation

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

7 Map analysis [i](#)

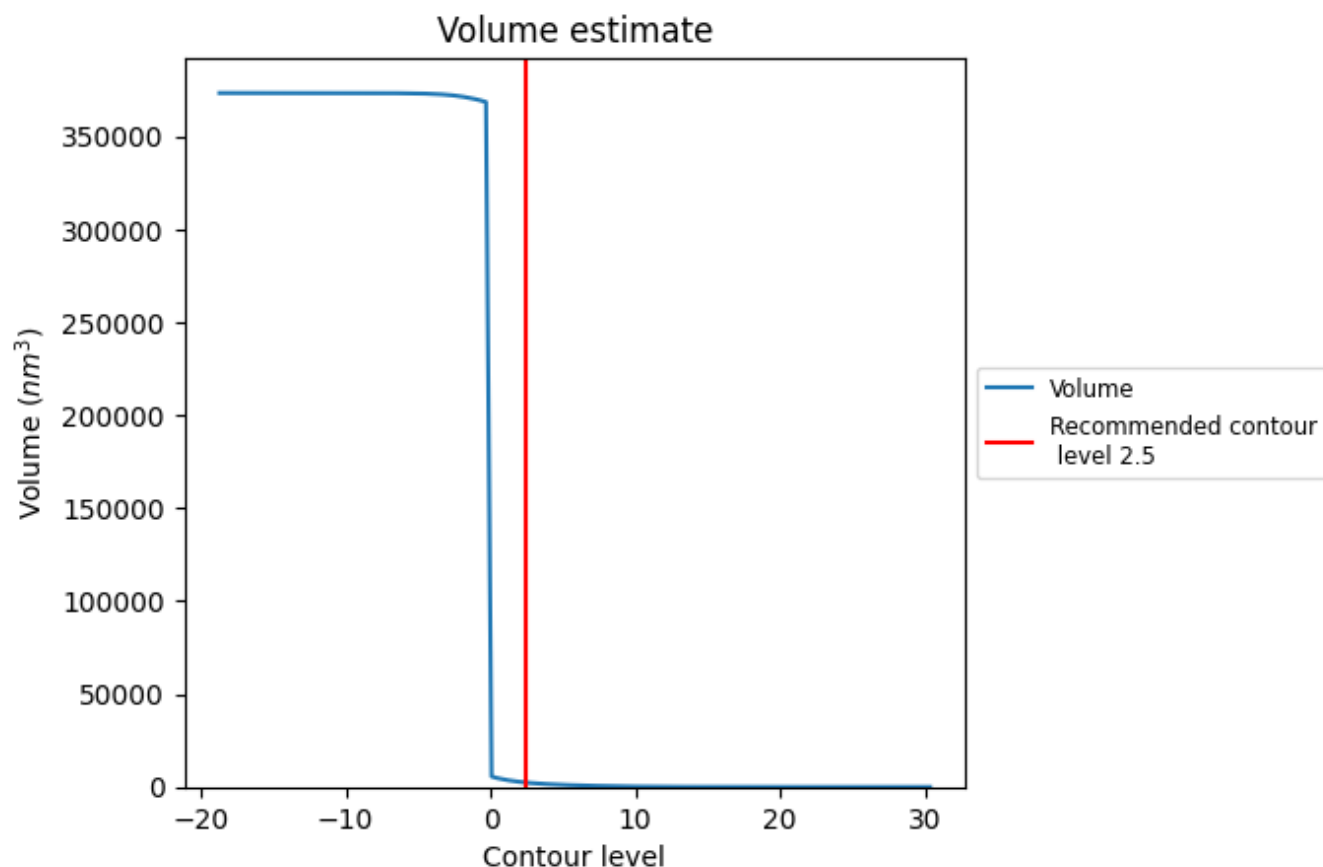
This section contains the results of statistical analysis of the map.

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.

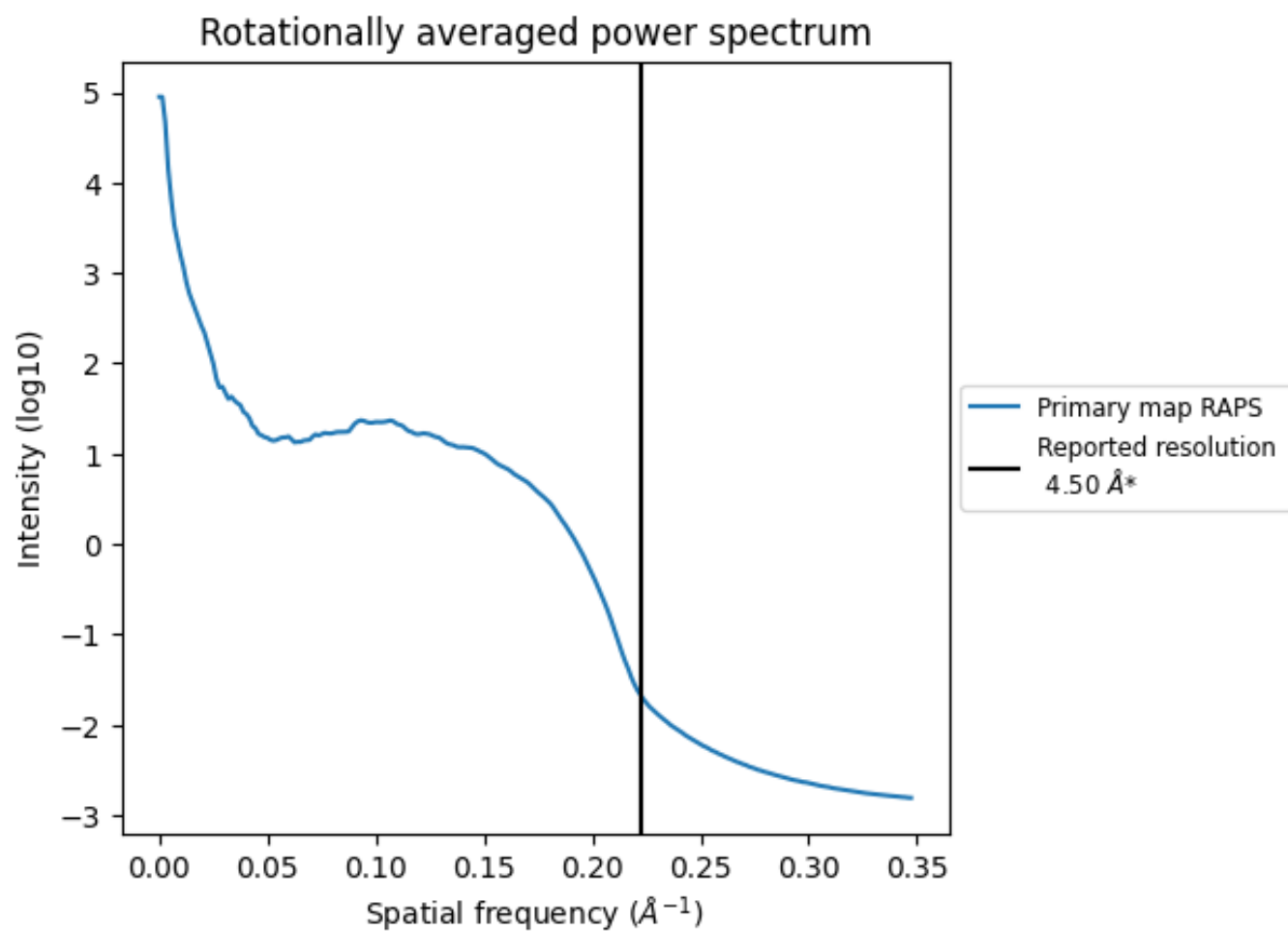
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2348 nm³; this corresponds to an approximate mass of 2121 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 0.222 Å⁻¹

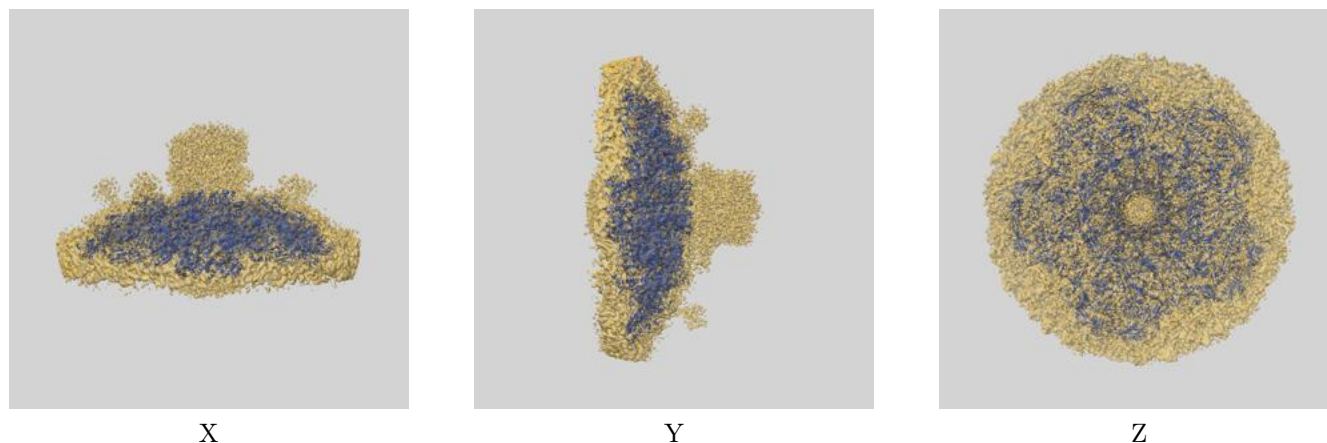
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

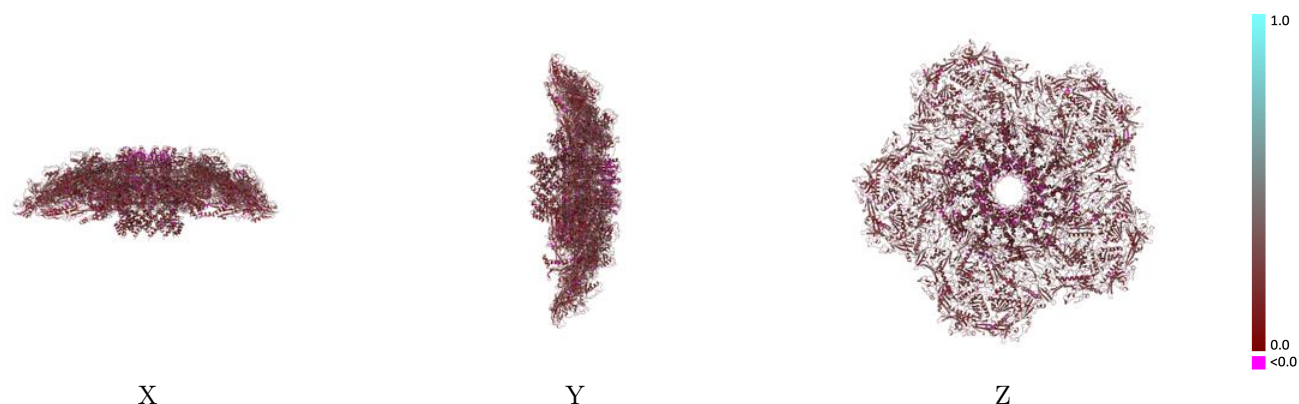
This section contains information regarding the fit between EMDB map EMD-20956 and PDB model 6UZC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



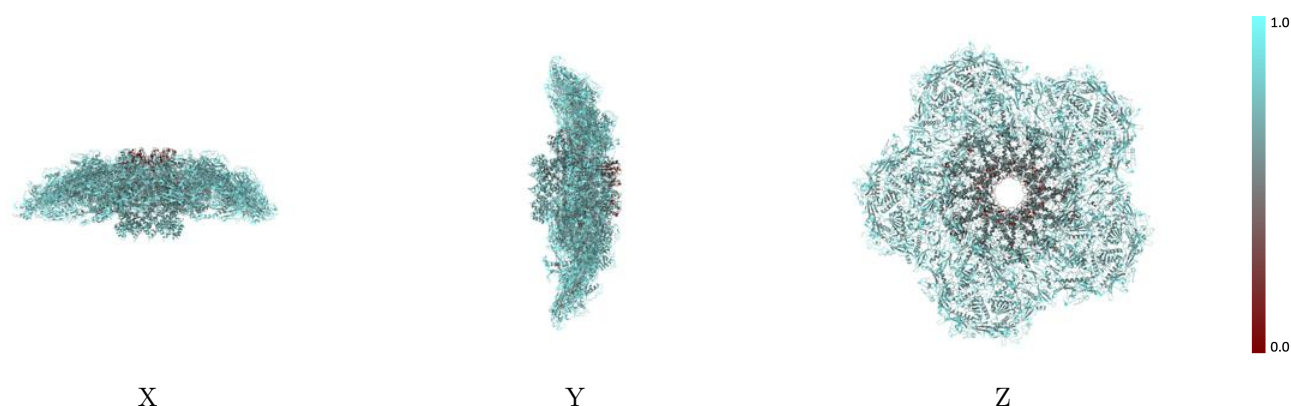
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



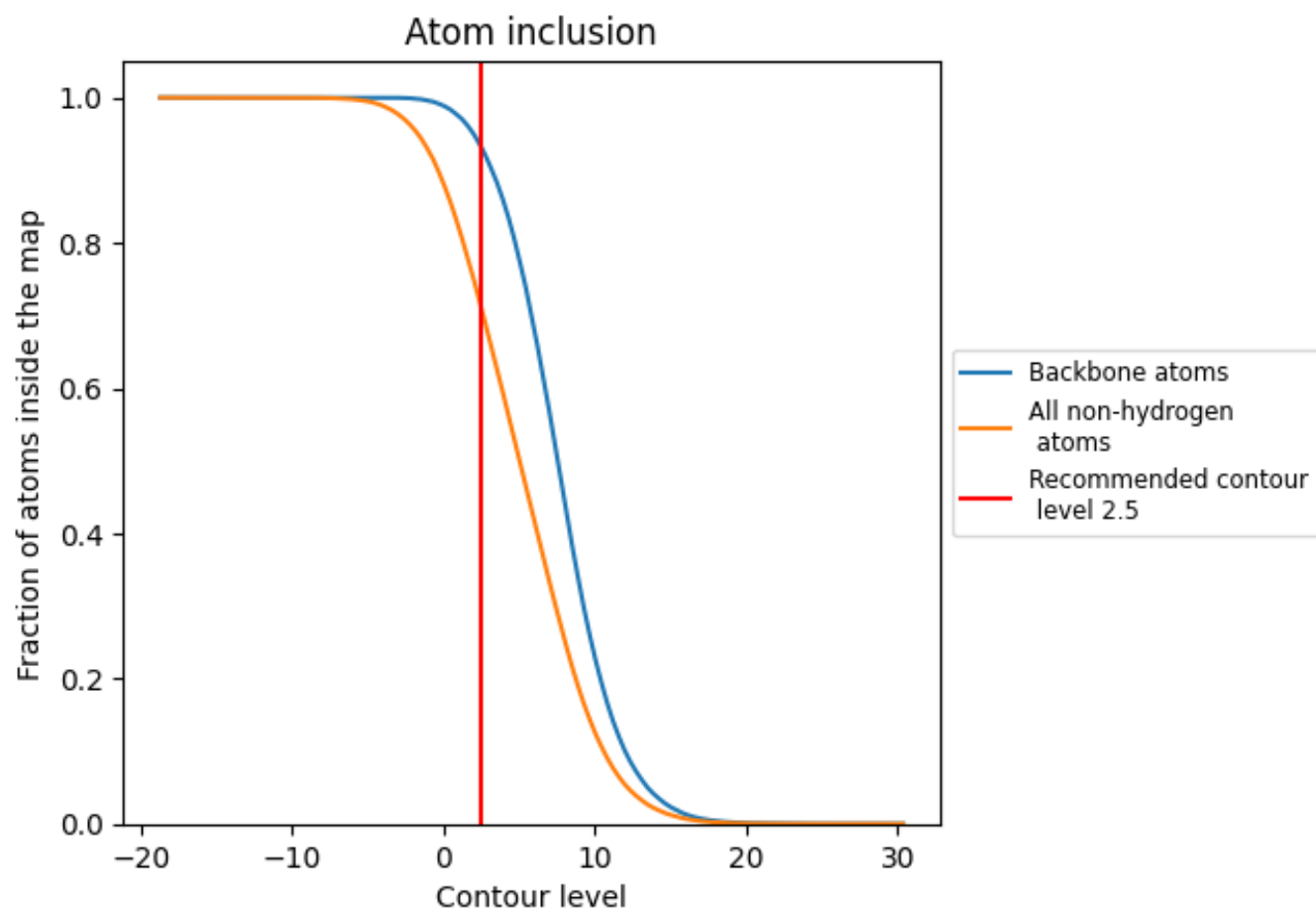
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 71% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.2320
A	 0.7450	 0.2370
B	 0.7514	 0.2490
C	 0.7575	 0.2630
D	 0.7585	 0.2680
E	 0.5949	 0.1820
F	 0.6132	 0.1870
G	 0.6212	 0.1930
H	 0.6222	 0.1920
I	 0.6193	 0.1920
J	 0.6160	 0.1840
K	 0.6142	 0.1870
L	 0.6164	 0.1990
M	 0.6261	 0.1940
N	 0.6281	 0.1840
O	 0.6145	 0.1870
P	 0.6121	 0.1900
a	 0.7707	 0.2590
b	 0.7547	 0.2430
c	 0.7404	 0.2350
d	 0.7651	 0.2500
e	 0.7550	 0.2620
f	 0.7599	 0.2680
g	 0.7591	 0.2570
h	 0.7553	 0.2400
i	 0.7502	 0.2380
j	 0.7645	 0.2550
k	 0.7610	 0.2590
l	 0.7541	 0.2680
m	 0.7565	 0.2590
n	 0.7459	 0.2440
o	 0.7431	 0.2340
p	 0.7597	 0.2500
q	 0.7644	 0.2580
r	 0.7576	 0.2640



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Chain	Atom inclusion	Q-score
s	 0.7565	 0.2590
t	 0.7556	 0.2400
u	 0.7538	 0.2430
v	 0.7568	 0.2440
w	 0.7591	 0.2640
x	 0.7547	 0.2670
y	 0.7606	 0.2600
z	 0.7470	 0.2400