



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:06 PM UTC

PDB ID : 5GAI / pdb_00005gai
EMDB ID : EMD-8005
Title : Probabilistic Structural Models of Mature P22 Bacteriophage Portal, Hub, and Tailspike proteins
Authors : Pintilie, G.; Chen, D.H.; Haase-Pettingell, C.A.; King, J.A.; Chiu, W.
Deposited on : 2015-12-01
Resolution : 10.50 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

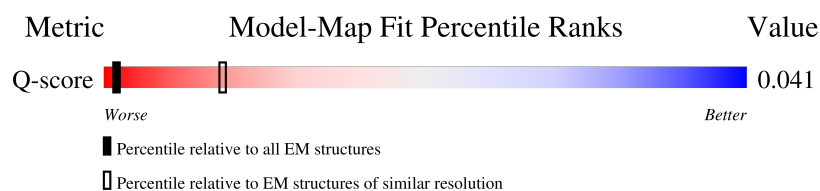
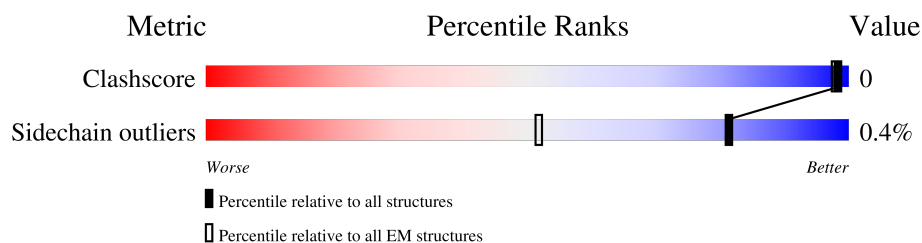
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

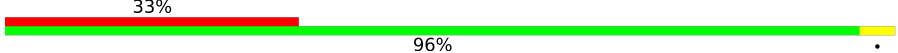
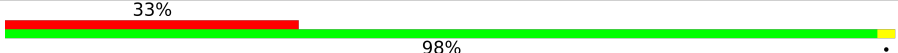
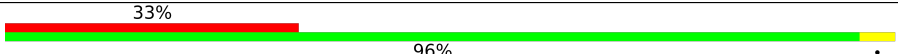
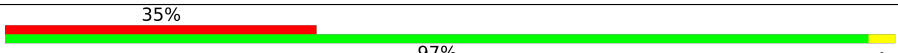
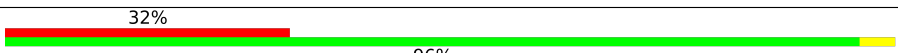
The reported resolution of this entry is 10.50 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	126 (10.00 - 11.00)

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	721	
1	B	721	
1	C	721	
1	D	721	
1	E	721	

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Mol	Chain	Length	Quality of chain
1	F	721	29% 97% .
1	G	721	30% 96% .
1	H	721	34% 97% .
1	I	721	32% 98% .
1	J	721	34% 96% .
1	W	721	33% 96% .
1	X	721	34% 98% .
2	K	146	29% 98% .
2	L	146	29% 97% .
2	M	146	33% 97% .
2	N	146	28% 97% .
2	O	146	32% 98% .
2	P	146	30% 98% .
2	Q	146	35% 97% .
2	R	146	37% 97% .
2	S	146	37% 97% .
2	T	146	33% 95% ..
2	U	146	26% 95% ..
2	V	146	29% 98% .
3	O	662	49% 96% .
3	Y	662	60% 94% 6%
3	Z	662	46% 99% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 98043 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	B	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	C	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	D	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	E	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	F	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	G	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	H	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	I	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	J	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	W	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		
1	X	721	Total	C	N	O	S	0	0
			5792	3622	1005	1141	24		

- Molecule 2 is a protein called Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	L	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	M	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	O	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	P	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	Q	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	R	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	S	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	T	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	U	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		
2	V	146	Total	C	N	O	S	0	0
			1122	704	192	221	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	150	PRO	ALA	engineered mutation	UNP P26746
L	150	PRO	ALA	engineered mutation	UNP P26746
M	150	PRO	ALA	engineered mutation	UNP P26746
N	150	PRO	ALA	engineered mutation	UNP P26746
O	150	PRO	ALA	engineered mutation	UNP P26746
P	150	PRO	ALA	engineered mutation	UNP P26746
Q	150	PRO	ALA	engineered mutation	UNP P26746
R	150	PRO	ALA	engineered mutation	UNP P26746
S	150	PRO	ALA	engineered mutation	UNP P26746
T	150	PRO	ALA	engineered mutation	UNP P26746
U	150	PRO	ALA	engineered mutation	UNP P26746
V	150	PRO	ALA	engineered mutation	UNP P26746

- Molecule 3 is a protein called Tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	662	Total	C	N	O	S	0	0
			5025	3169	855	985	16		
3	Z	662	Total	C	N	O	S	0	0
			5025	3169	855	985	16		

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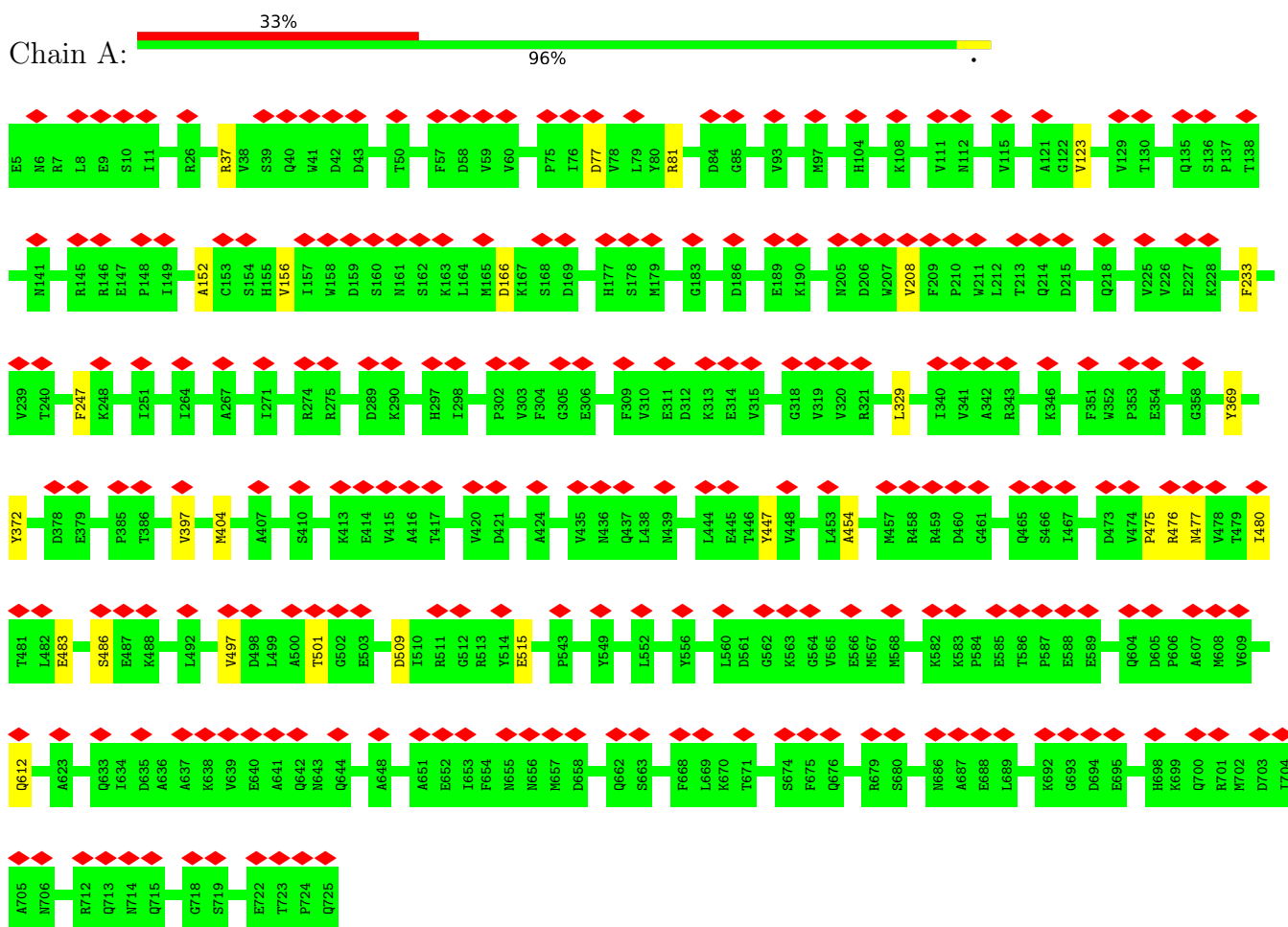
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	0	662	5025	3169	855	985	16	0	0

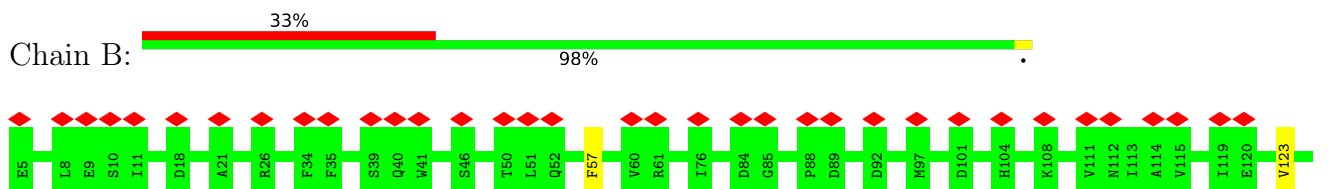
3 Residue-property plots

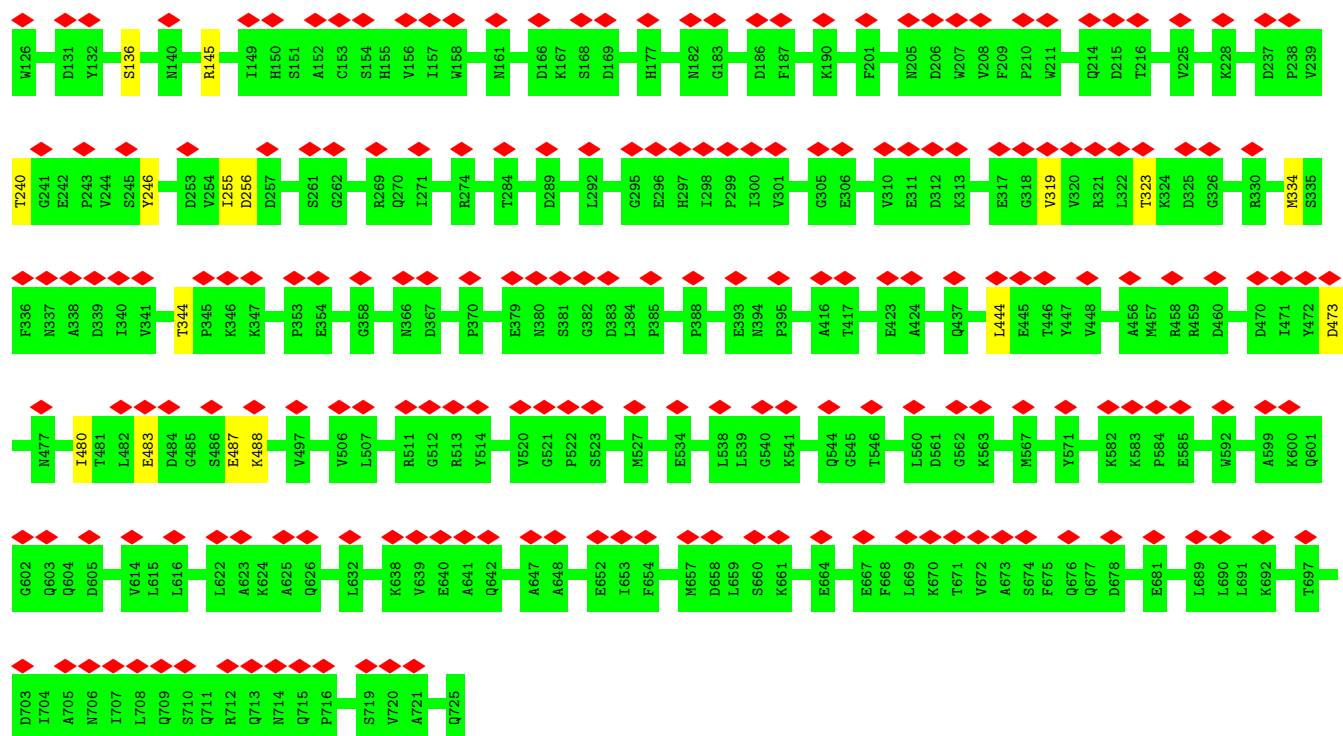
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Portal protein

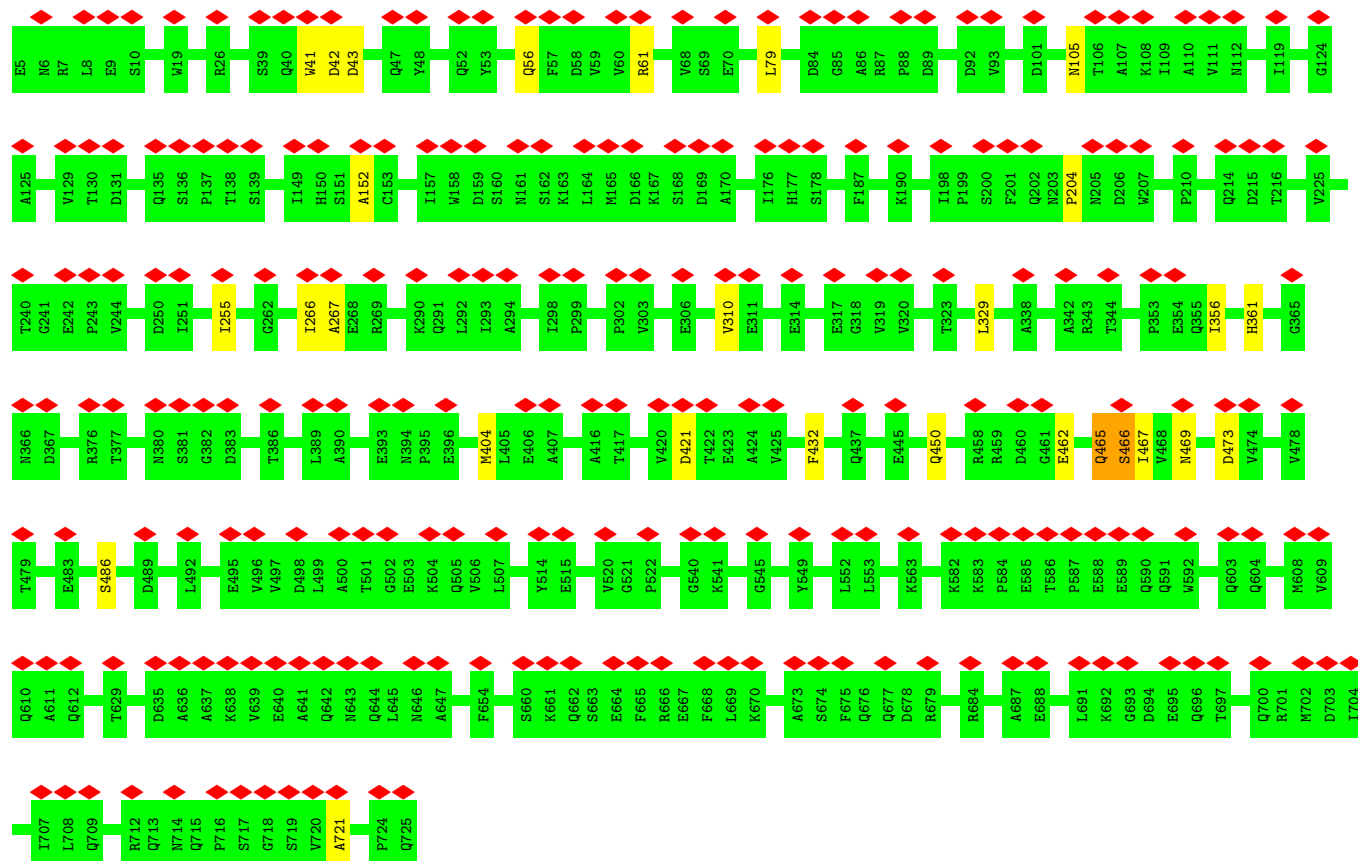


• Molecule 1: Portal protein

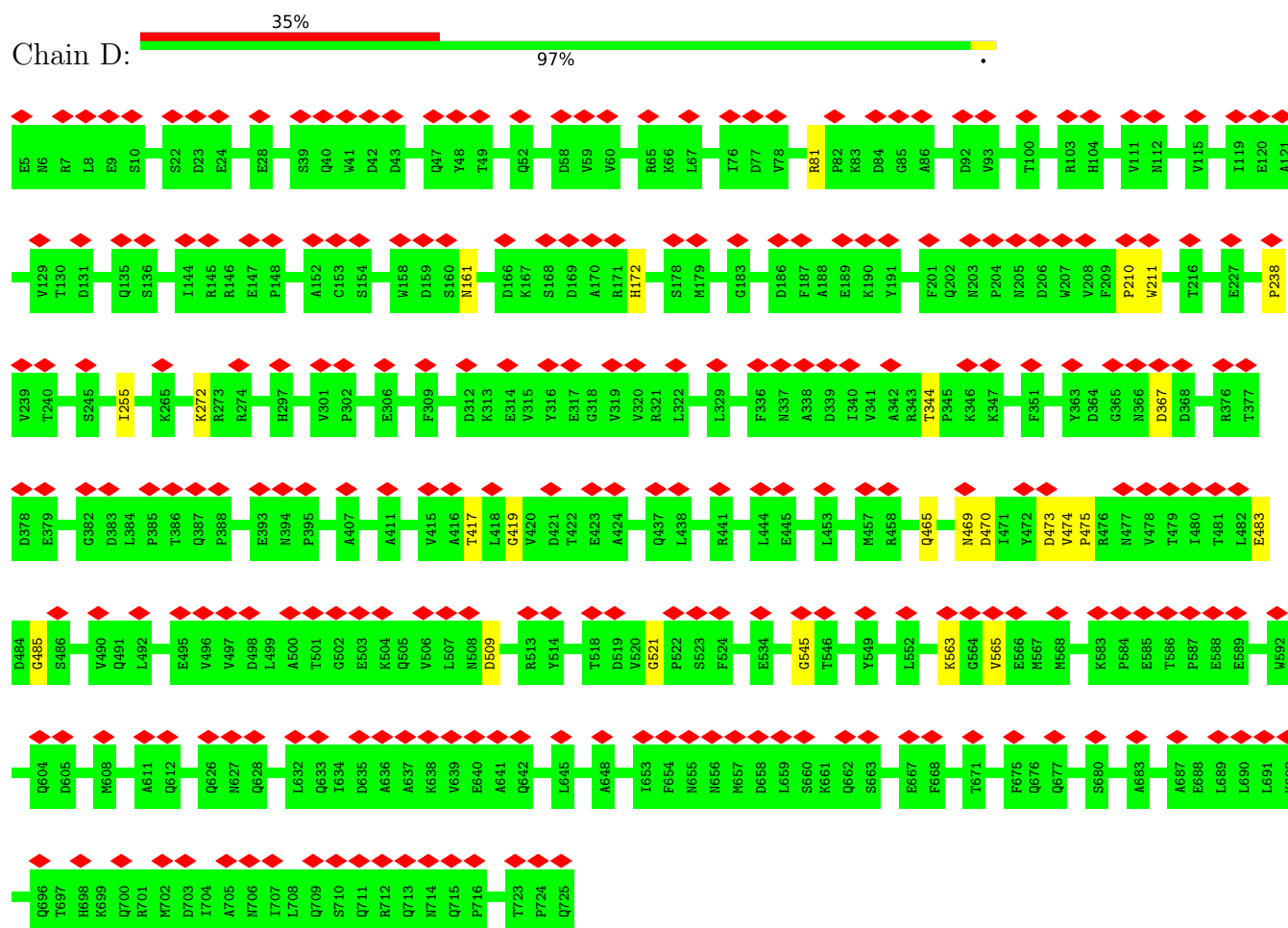




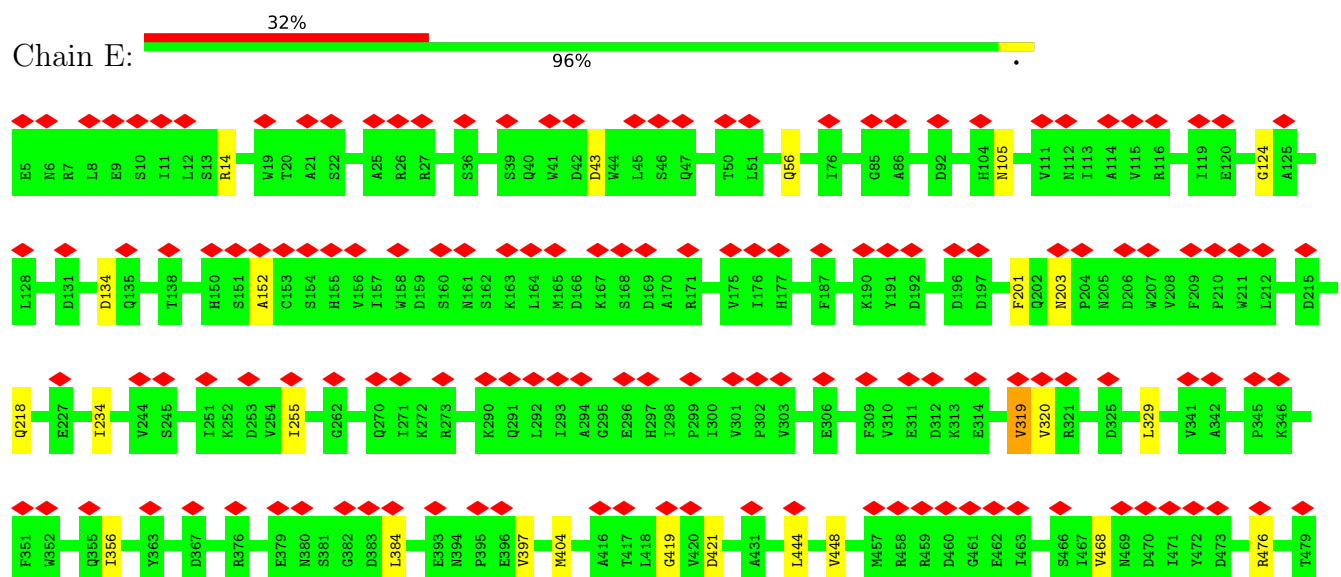
• Molecule 1: Portal protein

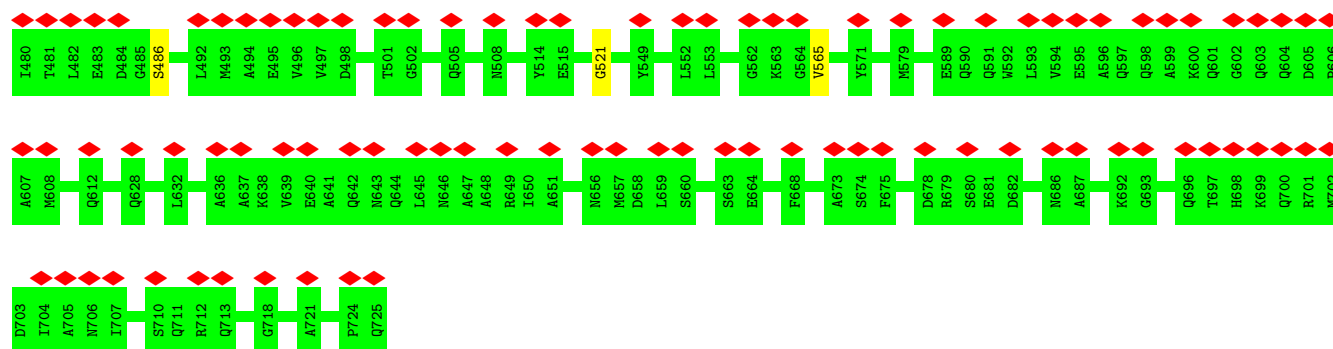


- Molecule 1: Portal protein

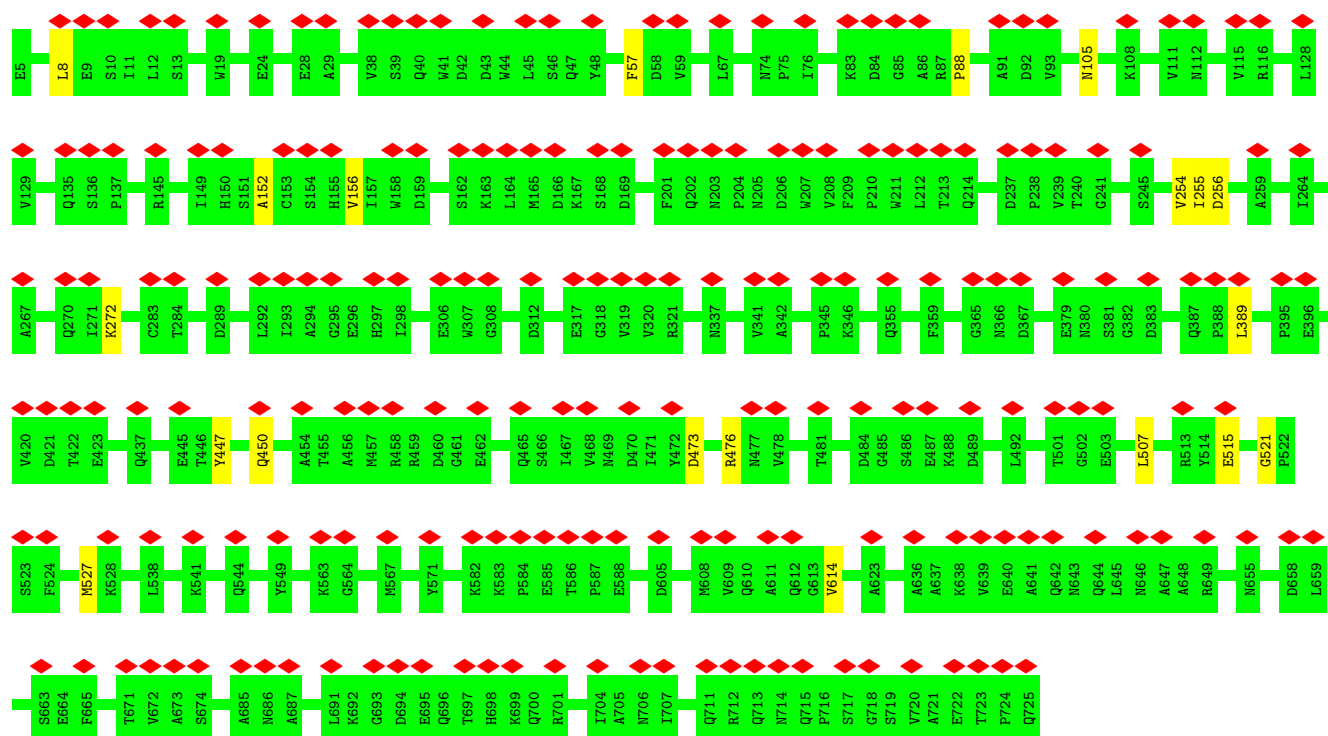


- Molecule 1: Portal protein

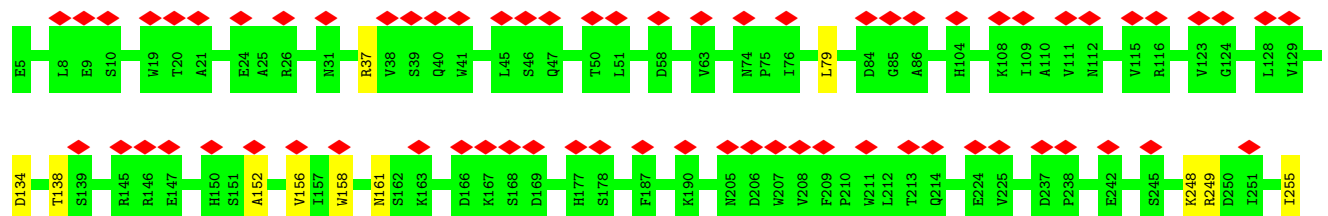


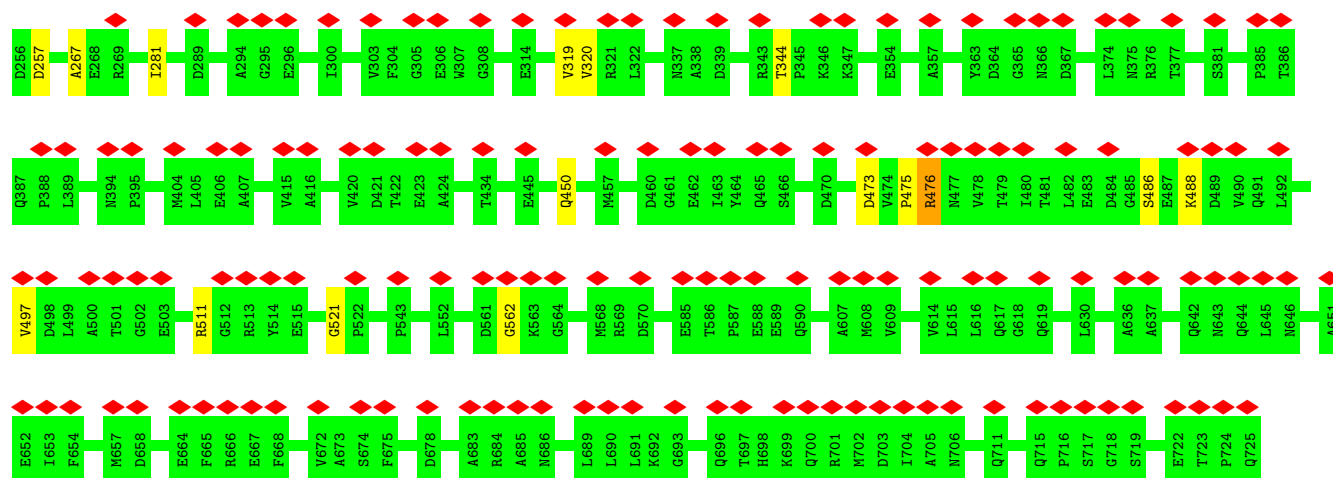


• Molecule 1: Portal protein

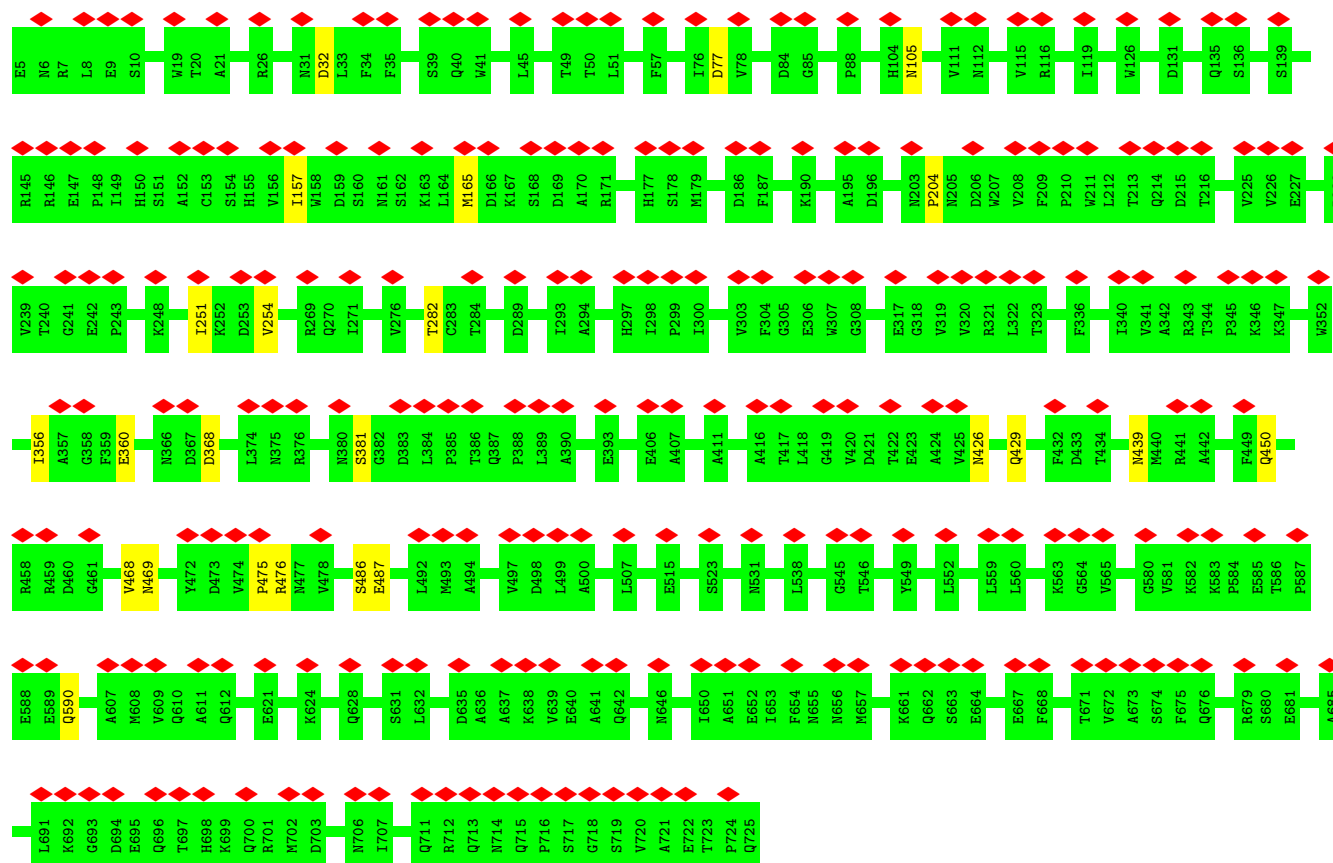


• Molecule 1: Portal protein



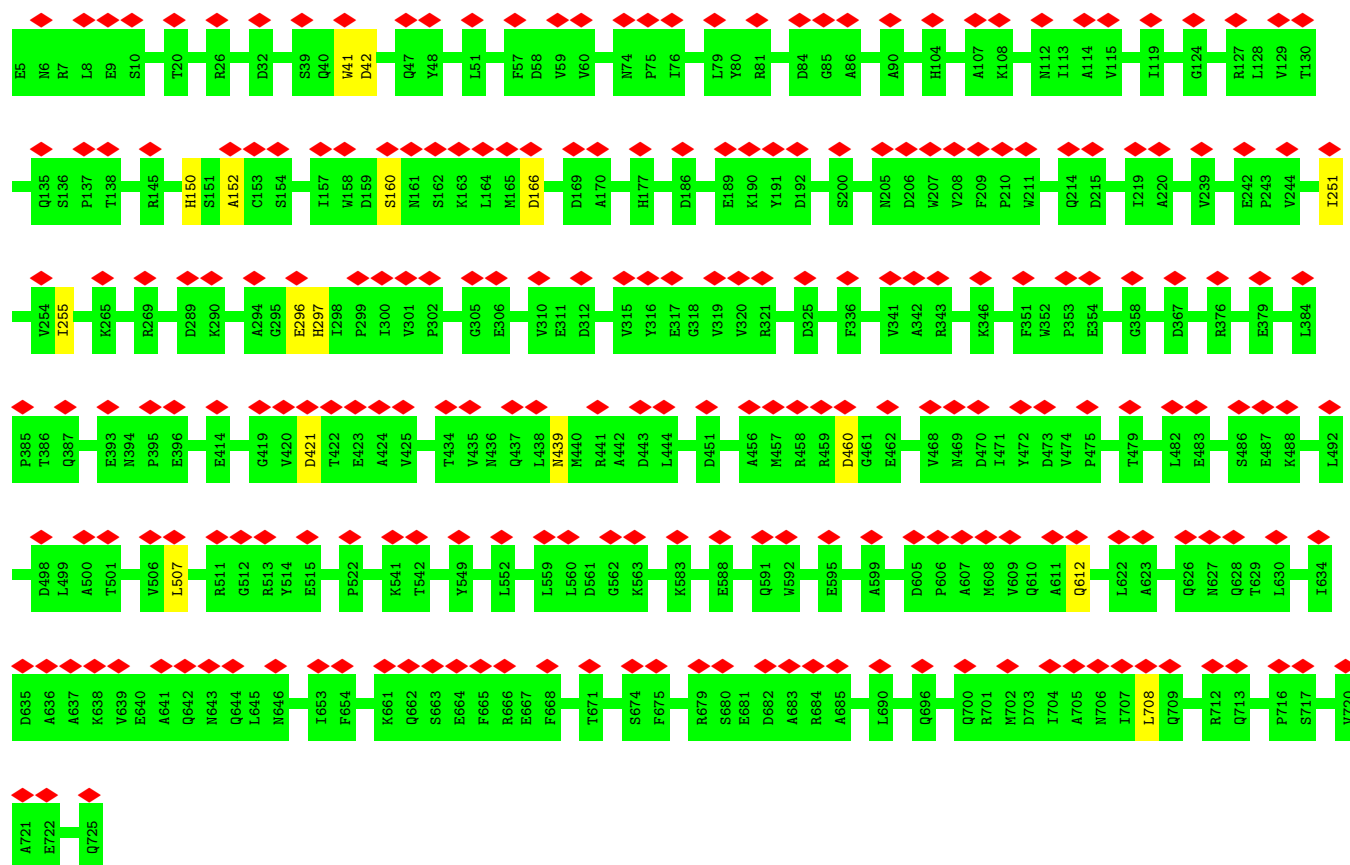


• Molecule 1: Portal protein

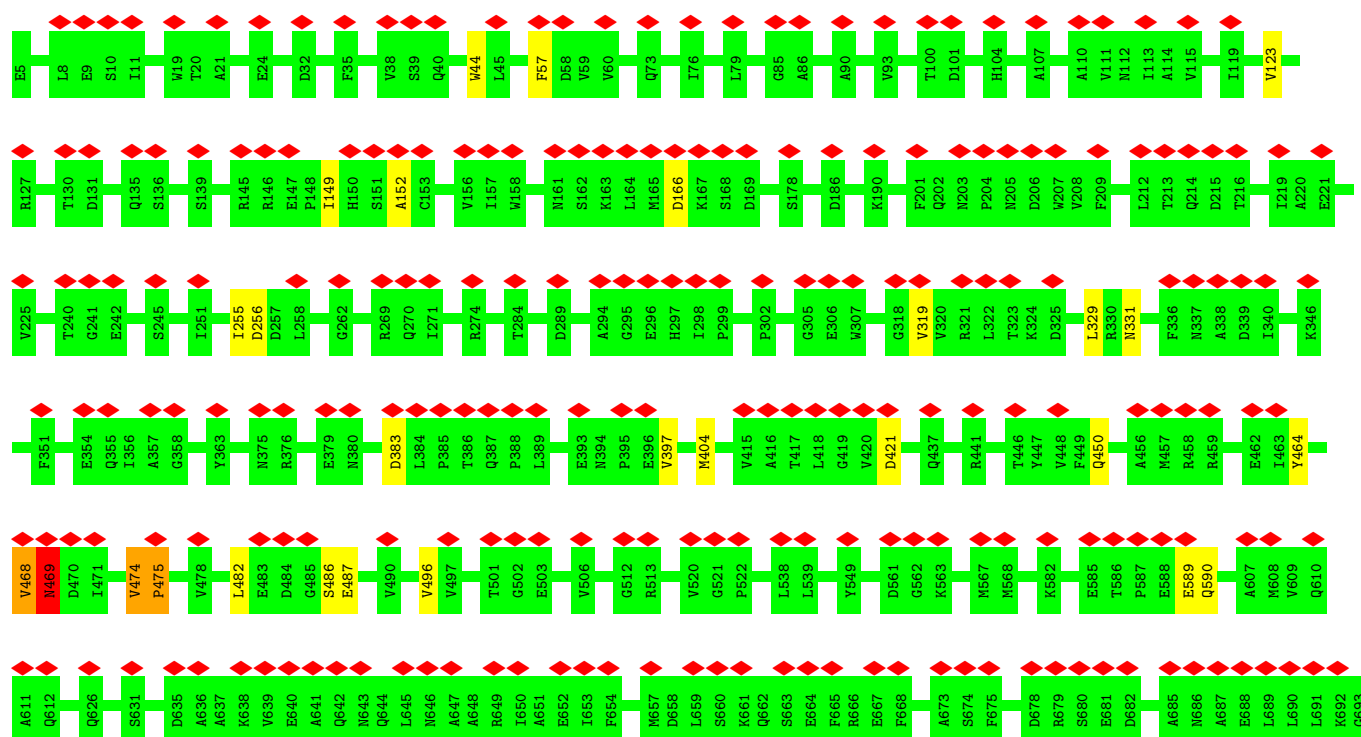


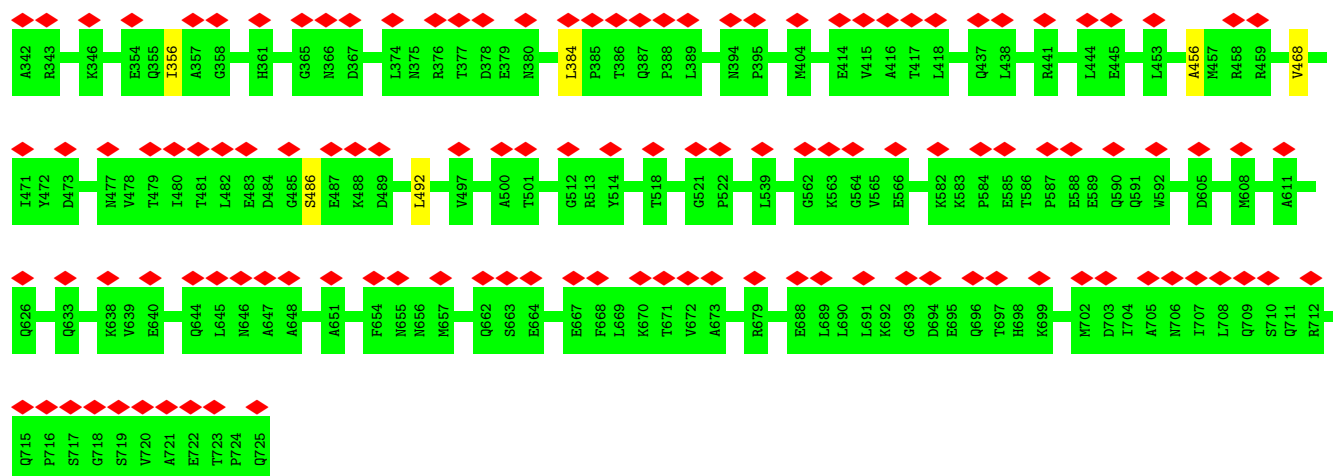
• Molecule 1: Portal protein





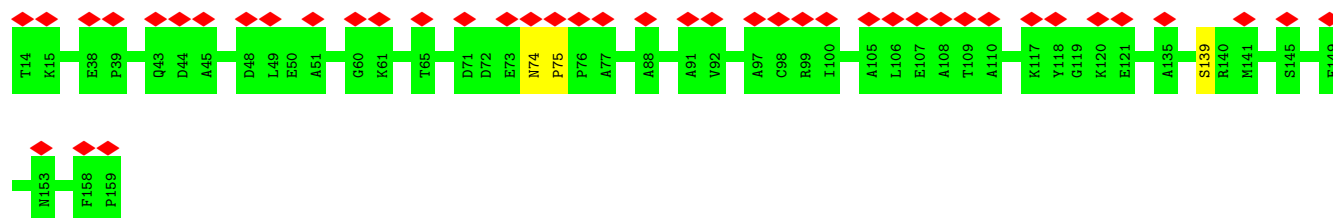
• Molecule 1: Portal protein





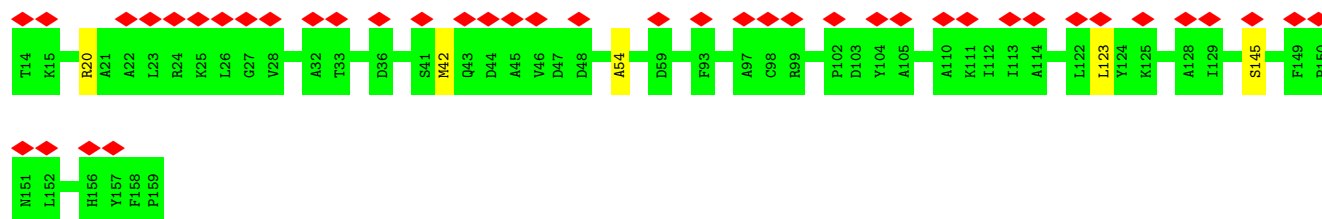
- Molecule 2: Peptidoglycan hydrolase gp4

Chain K: 29% 98%



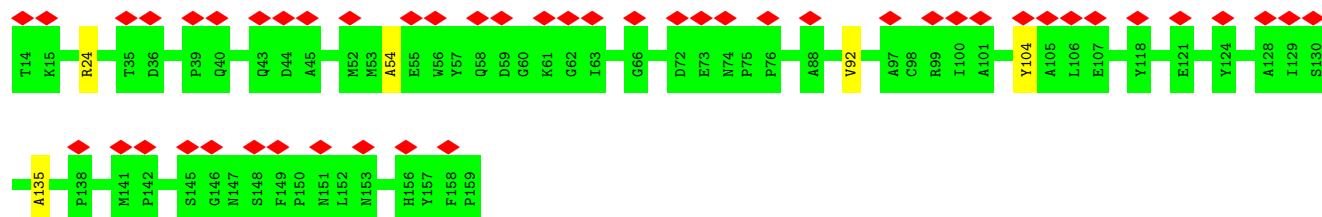
- Molecule 2: Peptidoglycan hydrolase gp4

Chain L: 29% 97%

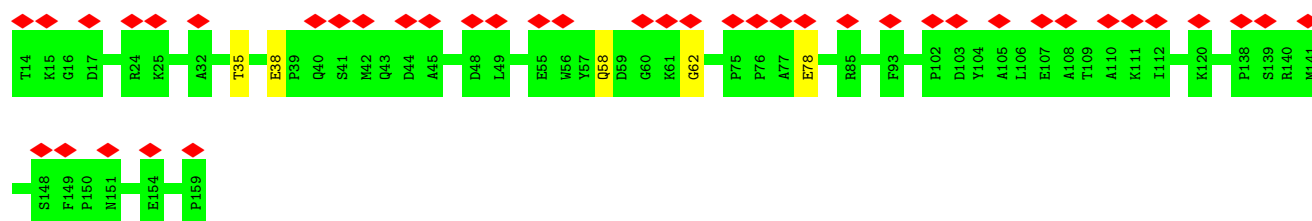


- Molecule 2: Peptidoglycan hydrolase gp4

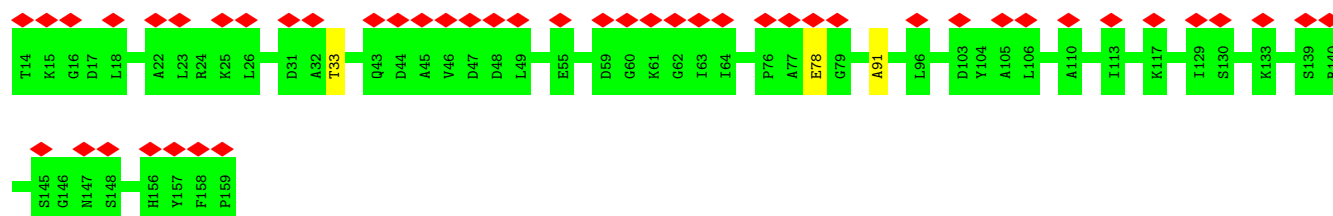
Chain M: 33% 97%



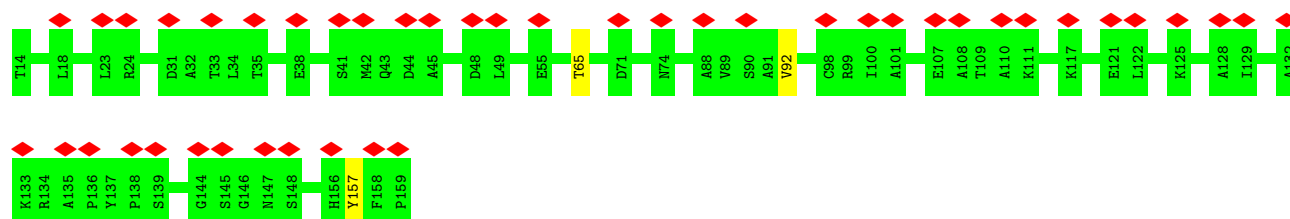
- Molecule 2: Peptidoglycan hydrolase gp4



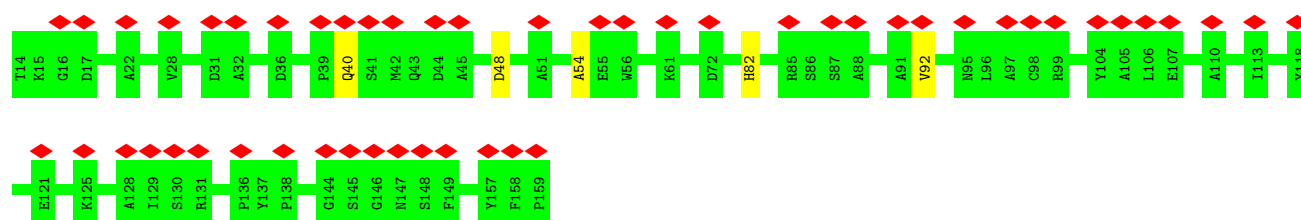
• Molecule 2: Peptidoglycan hydrolase gp4



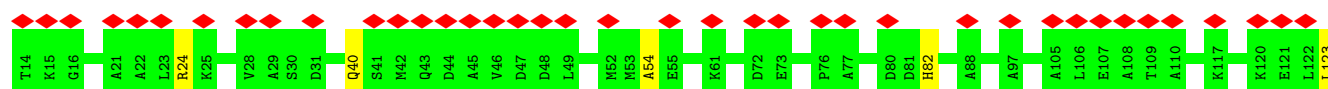
• Molecule 2: Peptidoglycan hydrolase gp4

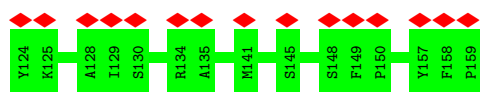


• Molecule 2: Peptidoglycan hydrolase gp4



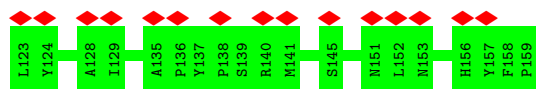
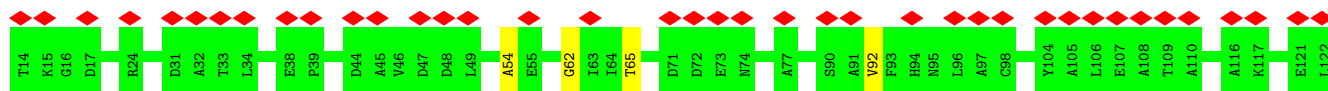
• Molecule 2: Peptidoglycan hydrolase gp4





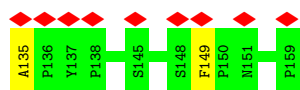
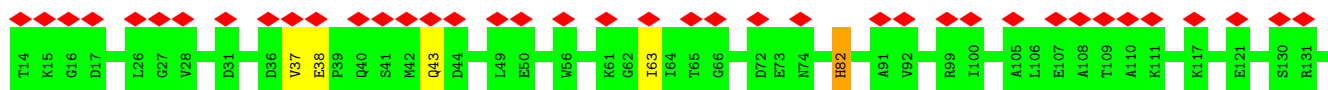
- Molecule 2: Peptidoglycan hydrolase gp4

Chain S: 37% 97%



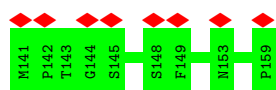
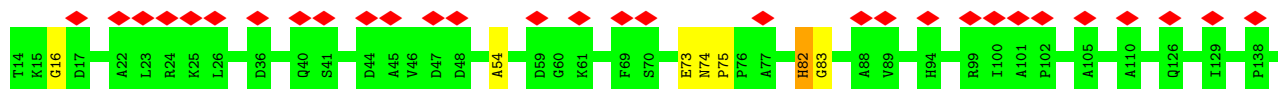
- Molecule 2: Peptidoglycan hydrolase gp4

Chain T: 33% 95%



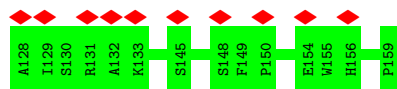
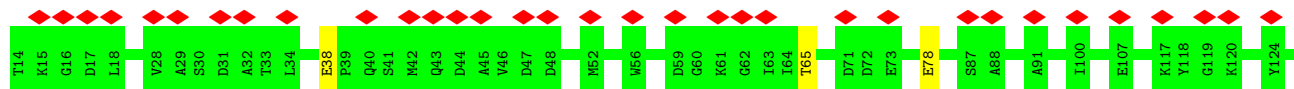
- Molecule 2: Peptidoglycan hydrolase gp4

Chain U: 26% 95%

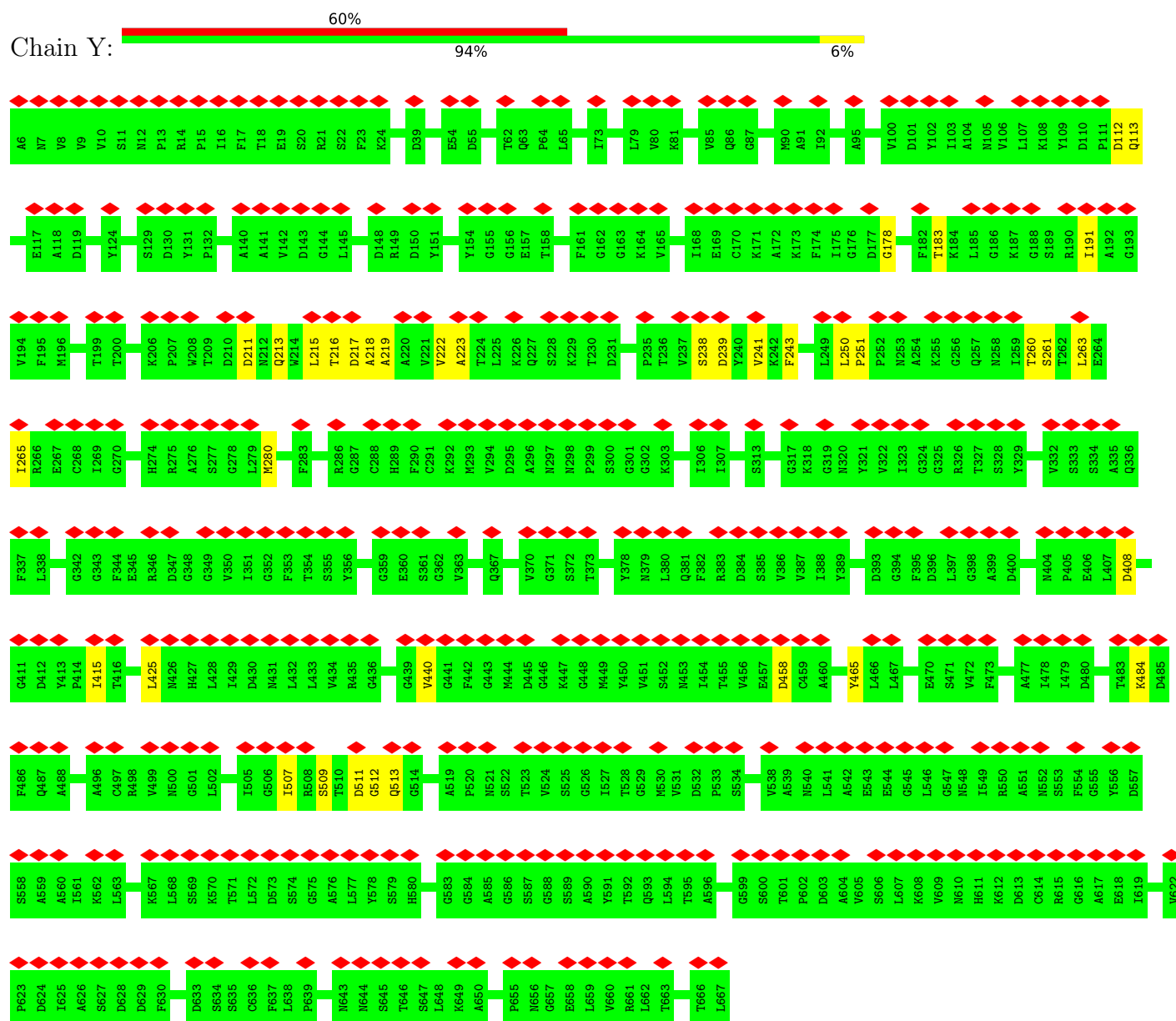


- Molecule 2: Peptidoglycan hydrolase gp4

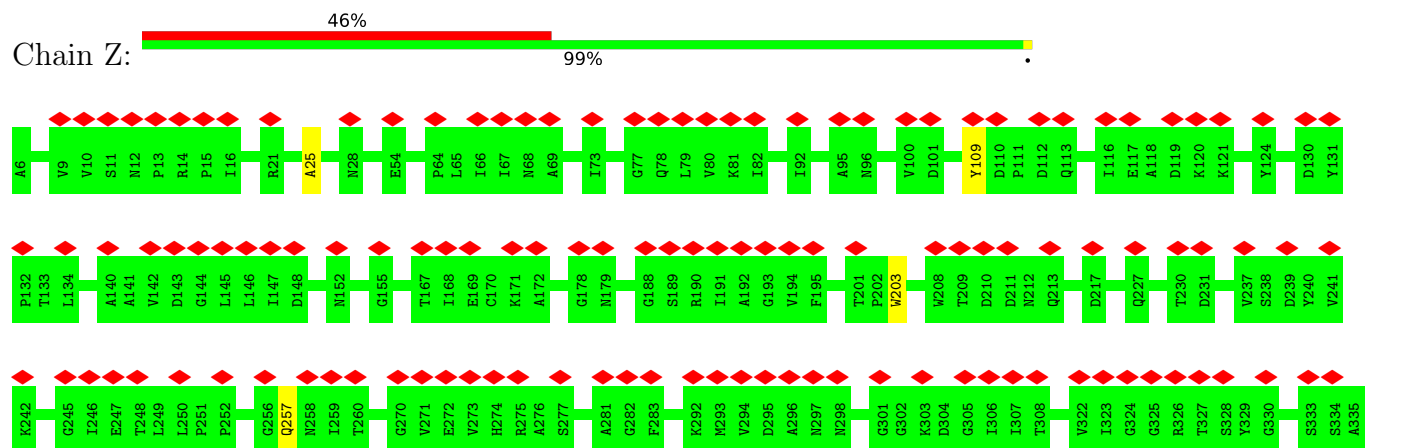
Chain V: 29% 98%

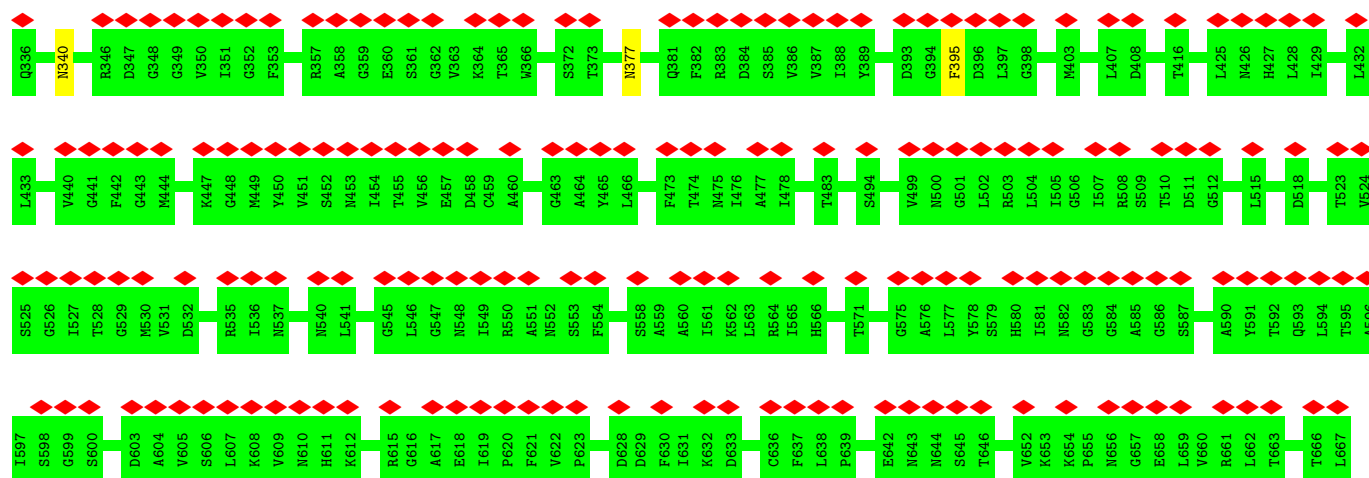


- Molecule 3: Tail fiber protein



• Molecule 3: Tail fiber protein





• Molecule 3: Tail fiber protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	70600	Depositor
Image detector	GATAN ULTRASCAN 10000 (10k x 10k)	Depositor
Maximum map value	1.469	Depositor
Minimum map value	-0.924	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	1305.6, 1305.6, 1305.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.55, 2.55, 2.55	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	1.18	0/5902	1.39	24/7997 (0.3%)
1	B	1.18	0/5902	1.39	13/7997 (0.2%)
1	C	1.19	1/5902 (0.0%)	1.41	16/7997 (0.2%)
1	D	1.18	0/5902	1.39	18/7997 (0.2%)
1	E	1.19	0/5902	1.39	17/7997 (0.2%)
1	F	1.19	0/5902	1.41	19/7997 (0.2%)
1	G	1.18	0/5902	1.41	20/7997 (0.3%)
1	H	1.19	0/5902	1.41	19/7997 (0.2%)
1	I	1.19	0/5902	1.39	13/7997 (0.2%)
1	J	1.19	0/5902	1.41	18/7997 (0.2%)
1	W	1.19	0/5902	1.39	17/7997 (0.2%)
1	X	1.19	0/5902	1.38	10/7997 (0.1%)
2	K	1.17	0/1148	1.45	0/1558
2	L	1.18	0/1148	1.53	3/1558 (0.2%)
2	M	1.15	0/1148	1.47	8/1558 (0.5%)
2	N	1.16	0/1148	1.48	6/1558 (0.4%)
2	O	1.15	0/1148	1.50	3/1558 (0.2%)
2	P	1.16	0/1148	1.49	4/1558 (0.3%)
2	Q	1.16	0/1148	1.47	6/1558 (0.4%)
2	R	1.16	0/1148	1.46	2/1558 (0.1%)
2	S	1.18	0/1148	1.50	7/1558 (0.4%)
2	T	1.18	1/1148 (0.1%)	1.50	6/1558 (0.4%)
2	U	1.16	0/1148	1.51	4/1558 (0.3%)
2	V	1.16	0/1148	1.47	2/1558 (0.1%)
3	O	1.21	0/5128	1.32	18/6966 (0.3%)
3	Y	1.20	0/5128	1.34	15/6966 (0.2%)
3	Z	1.21	0/5128	1.30	1/6966 (0.0%)
All	All	1.19	2/99984 (0.0%)	1.40	289/135558 (0.2%)

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	A	0	6
1	B	0	1
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	3
1	G	0	4
1	H	0	5
1	J	0	8
1	W	0	4
1	X	0	2
2	K	0	1
2	U	0	1
2	V	0	1
3	O	0	9
3	Y	0	17
3	Z	0	1
All	All	0	78

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	721	ALA	CA-C	-5.32	1.50	1.53
2	T	149	PHE	CA-CB	5.09	1.56	1.52

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	ASP	CA-C-N	10.11	126.61	120.24
1	B	473	ASP	C-N-CA	10.11	126.61	120.24
1	G	473	ASP	CA-C-N	9.45	126.19	120.24
1	G	473	ASP	C-N-CA	9.45	126.19	120.24
1	H	251	ILE	N-CA-C	-8.94	105.22	113.71
3	Y	222	VAL	N-CA-C	-8.87	104.50	113.10
1	F	254	VAL	N-CA-C	-8.47	103.52	111.48
2	O	78	GLU	N-CA-C	-8.09	104.56	114.75
2	S	65	THR	N-CA-C	-8.02	105.48	114.62
1	I	251	ILE	N-CA-C	-7.61	105.35	112.96
2	L	54	ALA	N-CA-C	-7.59	105.97	114.62
1	W	57	PHE	N-CA-C	-7.53	106.04	114.62
1	J	383	ASP	N-CA-C	-7.53	106.04	114.62
3	O	368	GLY	N-CA-C	-7.38	103.53	111.21
3	O	516	THR	N-CA-C	-7.38	104.14	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	57	PHE	N-CA-C	-7.27	104.27	113.43
2	R	54	ALA	N-CA-C	-7.21	106.40	114.62
3	O	415	ILE	N-CA-C	-7.04	106.27	113.10
3	Y	251	PRO	CA-C-O	-7.00	115.86	120.90
2	V	65	THR	N-CA-C	-6.96	105.97	114.75
1	E	234	ILE	N-CA-C	-6.96	99.16	108.35
2	P	65	THR	N-CA-C	-6.96	106.69	114.62
3	O	484	LYS	N-CA-C	-6.88	106.08	114.75
1	J	421	ASP	N-CA-C	-6.83	106.15	114.75
2	S	54	ALA	CA-C-N	6.67	129.55	120.54
2	S	54	ALA	C-N-CA	6.67	129.55	120.54
1	A	497	VAL	N-CA-C	-6.62	105.67	113.42
1	C	450	GLN	CA-C-N	6.61	129.43	120.38
1	C	450	GLN	C-N-CA	6.61	129.43	120.38
1	J	469	ASN	CA-CB-CG	6.60	119.20	112.60
1	F	473	ASP	CA-C-N	6.50	125.53	120.33
1	F	473	ASP	C-N-CA	6.50	125.53	120.33
1	C	105	ASN	CA-CB-CG	-6.49	106.11	112.60
2	Q	54	ALA	N-CA-C	-6.48	107.23	114.62
2	P	157	TYR	CA-C-N	6.42	128.12	120.09
2	P	157	TYR	C-N-CA	6.42	128.12	120.09
1	A	486	SER	N-CA-C	-6.37	105.27	114.12
2	M	104	TYR	N-CA-C	-6.34	103.72	112.03
1	E	521	GLY	CA-C-N	6.31	126.33	119.89
1	E	521	GLY	C-N-CA	6.31	126.33	119.89
1	C	473	ASP	CA-C-N	6.29	125.36	120.33
1	C	473	ASP	C-N-CA	6.29	125.36	120.33
1	B	480	ILE	N-CA-C	-6.28	106.87	112.90
1	E	421	ASP	N-CA-C	-6.27	106.60	114.56
1	D	473	ASP	CA-C-N	6.25	125.33	120.33
1	D	473	ASP	C-N-CA	6.25	125.33	120.33
3	Y	241	VAL	N-CA-C	-6.24	107.05	113.10
1	I	612	GLN	CA-C-N	6.23	126.89	119.98
1	I	612	GLN	C-N-CA	6.23	126.89	119.98
2	Q	92	VAL	N-CA-C	6.20	116.37	110.42
3	O	456	VAL	N-CA-C	-6.13	99.66	108.42
2	M	92	VAL	N-CA-C	6.12	116.30	110.42
3	Y	250	LEU	CA-C-N	6.10	124.12	119.66
3	Y	250	LEU	C-N-CA	6.10	124.12	119.66
1	J	450	GLN	CA-C-N	6.07	128.41	120.28
1	J	450	GLN	C-N-CA	6.07	128.41	120.28
1	G	319	VAL	N-CA-C	-6.06	106.41	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	462	GLU	CA-C-N	6.05	128.75	120.35
1	C	462	GLU	C-N-CA	6.05	128.75	120.35
1	H	469	ASN	CA-CB-CG	6.04	118.64	112.60
3	Y	223	ALA	N-CA-C	-5.99	105.93	113.72
1	I	460	ASP	CA-C-N	5.97	125.78	120.10
1	I	460	ASP	C-N-CA	5.97	125.78	120.10
2	N	62	GLY	CA-C-N	5.97	128.51	120.50
2	N	62	GLY	C-N-CA	5.97	128.51	120.50
1	J	57	PHE	N-CA-C	-5.97	103.95	112.13
2	N	58	GLN	N-CA-C	-5.93	107.86	114.62
1	D	474	VAL	CA-C-O	-5.90	114.74	118.69
3	Y	465	TYR	N-CA-C	-5.90	99.73	108.99
1	D	563	LYS	N-CA-C	-5.89	103.65	111.96
1	J	152	ALA	CA-C-N	5.89	128.49	120.54
1	J	152	ALA	C-N-CA	5.89	128.49	120.54
3	O	478	ILE	N-CA-C	-5.88	99.58	108.17
1	W	404	MET	CG-SD-CE	-5.88	87.97	100.90
2	V	78	GLU	N-CA-C	-5.86	107.12	114.56
1	D	521	GLY	CA-C-N	5.85	125.86	119.89
1	D	521	GLY	C-N-CA	5.85	125.86	119.89
3	Y	425	LEU	N-CA-C	-5.84	106.70	113.88
1	H	204	PRO	N-CA-C	-5.82	108.00	114.92
1	A	612	GLN	CA-C-N	5.80	127.39	120.14
1	A	612	GLN	C-N-CA	5.80	127.39	120.14
3	Z	395	PHE	CA-CB-CG	-5.79	108.01	113.80
1	H	356	ILE	N-CA-C	-5.78	107.11	112.43
1	D	367	ASP	N-CA-C	-5.77	105.55	112.59
1	X	356	ILE	N-CA-C	-5.77	107.50	113.10
1	X	384	LEU	CA-C-N	5.77	125.77	119.89
1	X	384	LEU	C-N-CA	5.77	125.77	119.89
1	C	79	LEU	N-CA-C	-5.75	106.60	113.97
2	S	92	VAL	N-CA-C	5.74	116.39	110.36
1	X	152	ALA	CA-C-N	5.71	127.94	120.28
1	X	152	ALA	C-N-CA	5.71	127.94	120.28
1	D	344	THR	CA-C-N	5.71	125.72	119.89
1	D	344	THR	C-N-CA	5.71	125.72	119.89
2	Q	40	GLN	N-CA-C	-5.71	106.23	113.43
1	F	152	ALA	CA-C-N	5.70	127.92	120.28
1	F	152	ALA	C-N-CA	5.70	127.92	120.28
2	M	54	ALA	CA-C-N	5.70	128.19	120.38
2	M	54	ALA	C-N-CA	5.70	128.19	120.38
2	L	145	SER	N-CA-C	-5.70	106.37	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	289	HIS	N-CA-C	-5.69	100.50	109.50
1	H	105	ASN	CA-CB-CG	-5.68	106.92	112.60
1	A	477	ASN	N-CA-CB	5.67	120.07	110.49
1	A	77	ASP	CA-C-N	5.67	128.16	120.63
1	A	77	ASP	C-N-CA	5.67	128.16	120.63
1	H	77	ASP	CA-C-N	5.66	128.09	120.50
1	H	77	ASP	C-N-CA	5.66	128.09	120.50
2	T	43	GLN	N-CA-C	-5.65	106.42	113.38
1	D	238	PRO	N-CA-C	-5.65	108.19	114.92
1	I	152	ALA	CA-C-N	5.65	128.17	120.54
1	I	152	ALA	C-N-CA	5.65	128.17	120.54
1	J	474	VAL	CA-C-N	5.61	126.85	119.84
1	J	474	VAL	C-N-CA	5.61	126.85	119.84
1	J	496	VAL	N-CA-C	-5.61	107.52	112.90
1	E	419	GLY	N-CA-C	-5.58	106.04	112.29
1	F	105	ASN	CA-CB-CG	-5.58	107.02	112.60
1	W	480	ILE	N-CA-C	-5.58	99.51	107.77
1	D	81	ARG	CA-C-N	5.57	125.58	119.89
1	D	81	ARG	C-N-CA	5.57	125.58	119.89
1	C	310	VAL	N-CA-C	-5.57	107.44	112.12
1	G	161	ASN	N-CA-CB	5.56	119.88	110.49
1	C	361	HIS	N-CA-C	-5.56	106.50	113.72
1	G	79	LEU	N-CA-C	-5.55	107.75	114.75
1	A	509	ASP	CA-C-N	5.55	128.07	120.35
1	A	509	ASP	C-N-CA	5.55	128.07	120.35
1	G	476	ARG	N-CA-CB	5.53	119.84	110.49
1	C	465	GLN	N-CA-C	-5.52	108.33	114.62
1	B	57	PHE	N-CA-C	-5.51	106.92	113.97
1	E	356	ILE	N-CA-C	-5.50	107.37	112.43
1	J	319	VAL	N-CA-C	-5.50	107.62	112.90
1	F	88	PRO	N-CA-C	-5.49	107.65	114.68
3	Y	216	THR	N-CA-C	-5.49	104.84	112.03
1	E	152	ALA	CA-C-N	5.48	127.63	120.28
1	E	152	ALA	C-N-CA	5.48	127.63	120.28
1	H	439	ASN	CA-CB-CG	-5.48	107.12	112.60
1	W	582	LYS	N-CA-C	-5.46	106.55	113.43
2	M	135	ALA	CA-C-N	5.46	125.45	119.89
2	M	135	ALA	C-N-CA	5.46	125.45	119.89
1	A	480	ILE	N-CA-C	-5.45	100.21	108.17
3	0	322	VAL	N-CA-C	-5.45	101.16	108.35
1	G	562	GLY	N-CA-C	-5.45	103.45	110.69
1	H	165	MET	CA-C-N	5.44	127.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	165	MET	C-N-CA	5.44	127.57	120.28
1	B	323	THR	CA-C-N	5.43	128.09	120.28
1	B	323	THR	C-N-CA	5.43	128.09	120.28
1	G	488	LYS	N-CA-C	-5.42	105.63	113.21
1	G	257	ASP	CA-CB-CG	5.41	118.00	112.60
2	T	37	VAL	N-CA-C	-5.41	107.03	112.17
1	E	319	VAL	N-CA-C	-5.40	107.54	113.43
1	G	450	GLN	CA-C-N	5.36	127.72	120.38
1	G	450	GLN	C-N-CA	5.36	127.72	120.38
1	G	521	GLY	CA-C-N	5.36	125.36	119.90
1	G	521	GLY	C-N-CA	5.36	125.36	119.90
1	W	512	GLY	CA-C-N	5.35	127.89	120.29
1	W	512	GLY	C-N-CA	5.35	127.89	120.29
2	Q	82	HIS	CA-CB-CG	5.35	119.15	113.80
1	W	312	ASP	N-CA-CB	5.35	119.53	110.49
1	J	590	GLN	N-CA-CB	5.35	119.53	110.49
1	H	381	SER	N-CA-CB	5.34	119.52	110.49
1	W	6	ASN	N-CA-C	-5.34	106.25	114.16
1	H	254	VAL	N-CA-C	-5.34	106.46	111.48
1	I	166	ASP	CA-CB-CG	5.34	117.94	112.60
1	G	249	ARG	N-CA-C	-5.33	108.54	114.62
1	J	397	VAL	CA-C-N	5.32	125.32	119.89
1	J	397	VAL	C-N-CA	5.32	125.32	119.89
1	A	501	THR	N-CA-CB	5.32	119.47	110.49
2	N	38	GLU	CA-C-N	5.31	125.31	119.89
2	N	38	GLU	C-N-CA	5.31	125.31	119.89
3	O	265	ILE	N-CA-C	-5.31	100.47	108.12
1	B	256	ASP	CA-CB-CG	5.31	117.91	112.60
2	M	24	ARG	CA-C-N	5.31	127.34	120.44
2	M	24	ARG	C-N-CA	5.31	127.34	120.44
1	A	152	ALA	CA-C-N	5.30	127.39	120.28
1	A	152	ALA	C-N-CA	5.30	127.39	120.28
1	H	368	ASP	CA-C-N	5.30	128.72	120.60
1	H	368	ASP	C-N-CA	5.30	128.72	120.60
1	I	439	ASN	CA-CB-CG	-5.30	107.30	112.60
1	A	166	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	488	LYS	N-CA-CB	5.29	119.43	110.49
1	D	509	ASP	CA-C-N	5.29	127.59	120.50
1	D	509	ASP	C-N-CA	5.29	127.59	120.50
2	N	78	GLU	N-CA-C	-5.29	108.08	114.75
1	W	249	ARG	N-CA-C	-5.29	106.72	114.39
1	D	210	PRO	CA-C-N	5.28	128.60	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	PRO	C-N-CA	5.28	128.60	121.05
1	E	124	GLY	N-CA-C	-5.28	106.94	111.95
1	F	527	MET	CA-C-N	5.27	127.34	120.28
1	F	527	MET	C-N-CA	5.27	127.34	120.28
2	L	42	MET	N-CA-C	-5.27	106.36	114.16
1	B	240	THR	N-CA-CB	5.26	119.39	110.49
1	H	32	ASP	CA-CB-CG	-5.26	107.34	112.60
1	A	233	PHE	CA-CB-CG	-5.26	108.54	113.80
1	J	166	ASP	CA-CB-CG	5.26	117.86	112.60
3	Y	191	ILE	N-CA-C	-5.26	100.49	108.17
1	F	156	VAL	N-CA-CB	5.25	116.84	110.95
1	J	256	ASP	N-CA-C	5.25	117.75	111.71
3	Y	265	ILE	N-CA-C	-5.25	100.81	108.99
1	A	454	ALA	CA-C-N	5.25	127.26	120.44
1	A	454	ALA	C-N-CA	5.25	127.26	120.44
1	C	204	PRO	N-CA-C	-5.24	107.97	114.68
1	A	515	GLU	N-CA-C	-5.23	105.63	113.89
1	H	282	THR	N-CA-C	-5.23	101.35	109.72
1	W	233	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	319	VAL	N-CA-C	-5.22	107.66	112.83
3	Y	263	LEU	N-CA-C	-5.22	100.90	109.40
2	P	92	VAL	N-CA-C	5.21	115.42	110.42
1	X	456	ALA	N-CA-CB	5.21	119.30	110.49
1	G	152	ALA	CA-C-N	5.21	127.51	120.38
1	G	152	ALA	C-N-CA	5.21	127.51	120.38
1	G	344	THR	CA-C-N	5.21	125.20	119.89
1	G	344	THR	C-N-CA	5.21	125.20	119.89
3	O	438	LEU	N-CA-C	-5.20	107.10	113.50
1	J	149	ILE	N-CA-C	-5.20	100.63	108.12
1	A	247	PHE	CA-C-N	5.20	128.60	120.75
1	A	247	PHE	C-N-CA	5.20	128.60	120.75
1	C	421	ASP	CA-CB-CG	-5.20	107.40	112.60
1	X	256	ASP	N-CA-C	5.20	117.69	111.71
1	W	545	GLY	CA-C-N	5.19	127.44	120.58
1	W	545	GLY	C-N-CA	5.19	127.44	120.58
1	E	397	VAL	CA-C-N	5.19	125.19	119.89
1	E	397	VAL	C-N-CA	5.19	125.19	119.89
2	R	40	GLN	N-CA-C	-5.19	106.90	114.12
1	W	215	ASP	N-CA-C	-5.19	99.88	108.75
1	H	590	GLN	N-CA-C	5.18	117.60	111.33
3	O	304	ASP	CA-C-N	5.18	124.89	119.92
3	O	304	ASP	C-N-CA	5.18	124.89	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	507	LEU	N-CA-CB	5.18	119.25	110.49
1	G	497	VAL	N-CA-C	-5.18	107.70	112.83
1	X	257	ASP	CA-CB-CG	5.18	117.78	112.60
3	0	465	TYR	N-CA-C	-5.18	100.58	108.76
1	X	166	ASP	CA-CB-CG	5.17	117.78	112.60
1	I	296	GLU	N-CA-C	-5.17	107.01	113.72
2	S	54	ALA	N-CA-C	-5.16	99.81	110.80
1	C	432	PHE	CA-CB-CG	5.15	118.95	113.80
1	I	421	ASP	N-CA-C	-5.14	105.02	113.50
2	S	62	GLY	CA-C-N	5.14	127.47	120.63
2	S	62	GLY	C-N-CA	5.14	127.47	120.63
2	U	16	GLY	CA-C-N	5.13	127.15	120.28
2	U	16	GLY	C-N-CA	5.13	127.15	120.28
1	A	397	VAL	CA-C-N	5.12	125.11	119.89
1	A	397	VAL	C-N-CA	5.12	125.11	119.89
1	F	256	ASP	CA-C-N	5.10	127.11	120.28
1	F	256	ASP	C-N-CA	5.10	127.11	120.28
3	Y	211	ASP	N-CA-C	-5.10	105.78	112.41
3	0	14	ARG	CA-C-N	5.10	125.09	119.89
3	0	14	ARG	C-N-CA	5.10	125.09	119.89
2	O	91	ALA	CA-C-N	5.10	127.44	120.46
2	O	91	ALA	C-N-CA	5.10	127.44	120.46
3	Y	113	GLN	N-CA-CB	5.10	119.10	110.49
1	E	201	PHE	CA-C-N	5.09	127.11	120.28
1	E	201	PHE	C-N-CA	5.09	127.11	120.28
1	I	160	SER	N-CA-C	-5.09	106.63	114.16
2	T	38	GLU	CA-C-N	5.09	124.87	119.28
2	T	38	GLU	C-N-CA	5.09	124.87	119.28
1	X	468	VAL	N-CA-CB	5.09	119.62	111.23
1	A	81	ARG	CA-C-N	5.08	125.08	119.90
1	A	81	ARG	C-N-CA	5.08	125.08	119.90
1	F	450	GLN	CA-C-N	5.08	127.33	120.38
1	F	450	GLN	C-N-CA	5.08	127.33	120.38
3	Y	215	LEU	N-CA-C	-5.07	101.60	109.72
1	D	470	ASP	N-CA-C	-5.07	106.40	112.59
1	E	384	LEU	CA-C-N	5.07	126.18	119.84
1	E	384	LEU	C-N-CA	5.07	126.18	119.84
1	F	521	GLY	CA-C-N	5.07	125.35	119.92
1	F	521	GLY	C-N-CA	5.07	125.35	119.92
1	E	105	ASN	CA-CB-CG	-5.07	107.53	112.60
2	Q	48	ASP	CA-C-N	5.07	127.32	120.38
2	Q	48	ASP	C-N-CA	5.07	127.32	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	THR	N-CA-C	-5.06	98.62	109.81
2	T	135	ALA	CA-C-N	5.06	126.17	119.84
2	T	135	ALA	C-N-CA	5.06	126.17	119.84
1	W	483	GLU	N-CA-CB	5.06	119.05	110.49
1	D	545	GLY	N-CA-C	-5.06	105.59	112.52
1	F	507	LEU	N-CA-CB	5.06	119.04	110.49
3	0	473	PHE	CA-CB-CG	-5.05	108.75	113.80
1	W	89	ASP	CA-C-N	5.05	127.05	120.28
1	W	89	ASP	C-N-CA	5.05	127.05	120.28
1	H	450	GLN	CA-C-N	5.04	127.75	120.38
1	H	450	GLN	C-N-CA	5.04	127.75	120.38
3	0	234	GLN	CA-C-N	5.04	125.04	119.90
3	0	234	GLN	C-N-CA	5.04	125.04	119.90
2	U	54	ALA	CA-C-N	5.04	127.29	120.38
2	U	54	ALA	C-N-CA	5.04	127.29	120.38
1	G	267	ALA	N-CA-C	-5.04	106.16	113.21
1	I	507	LEU	N-CA-CB	5.03	118.98	110.49
1	B	487	GLU	CA-C-N	5.03	131.14	121.54
1	B	487	GLU	C-N-CA	5.03	131.14	121.54
1	C	61	ARG	CA-C-O	-5.01	113.48	118.34
1	C	356	ILE	N-CA-C	-5.01	108.09	112.90
1	F	515	GLU	N-CA-C	-5.01	105.23	113.50

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	0	113	GLN	Peptide
3	0	312	LEU	Peptide
3	0	401	THR	Peptide
3	0	402	ASP	Peptide
3	0	406	GLU	Peptide
3	0	412	ASP	Peptide
3	0	419	PRO	Peptide
3	0	445	ASP	Peptide
3	0	450	TYR	Sidechain
1	A	369	TYR	Sidechain
1	A	372	TYR	Sidechain
1	A	447	TYR	Sidechain
1	A	475	PRO	Peptide
1	A	476	ARG	Peptide
1	A	483	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	483	GLU	Peptide
1	C	152	ALA	Peptide
1	C	465	GLN	Peptide
1	C	466	SER	Peptide
1	C	469	ASN	Peptide
1	C	486	SER	Peptide
1	D	465	GLN	Peptide
1	D	469	ASN	Peptide
1	D	475	PRO	Peptide
1	D	483	GLU	Peptide
1	D	485	GLY	Peptide
1	E	14	ARG	Sidechain
1	E	319	VAL	Peptide
1	E	468	VAL	Peptide
1	E	476	ARG	Peptide
1	E	486	SER	Peptide
1	F	447	TYR	Sidechain
1	F	476	ARG	Peptide
1	F	8	LEU	Peptide
1	G	158	TRP	Peptide
1	G	37	ARG	Sidechain
1	G	475	PRO	Peptide
1	G	486	SER	Peptide
1	H	468	VAL	Peptide
1	H	475	PRO	Peptide
1	H	476	ARG	Peptide
1	H	486	SER	Peptide
1	H	487	GLU	Peptide
1	J	464	TYR	Sidechain
1	J	468	VAL	Peptide
1	J	474	VAL	Peptide
1	J	475	PRO	Peptide
1	J	482	LEU	Peptide
1	J	486	SER	Peptide
1	J	487	GLU	Peptide
1	J	589	GLU	Peptide
2	K	139	SER	Peptide
2	U	73	GLU	Peptide
2	V	38	GLU	Peptide
1	W	476	ARG	Peptide
1	W	482	LEU	Peptide
1	W	492	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	W	587	PRO	Peptide
1	X	486	SER	Peptide
1	X	492	LEU	Peptide
3	Y	112	ASP	Peptide
3	Y	178	GLY	Peptide
3	Y	213	GLN	Peptide
3	Y	217	ASP	Peptide
3	Y	218	ALA	Peptide
3	Y	219	ALA	Peptide
3	Y	238	SER	Peptide
3	Y	239	ASP	Peptide
3	Y	243	PHE	Peptide
3	Y	280	MET	Peptide
3	Y	458	ASP	Peptide
3	Y	484	LYS	Peptide
3	Y	507	ILE	Peptide
3	Y	509	SER	Peptide
3	Y	511	ASP	Peptide
3	Y	512	GLY	Peptide
3	Y	513	GLN	Peptide
3	Z	109	TYR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5792	0	5623	3	0
1	B	5792	0	5623	2	0
1	C	5792	0	5623	6	0
1	D	5792	0	5623	5	0
1	E	5792	0	5623	5	0
1	F	5792	0	5623	2	0
1	G	5792	0	5623	3	0
1	H	5792	0	5623	1	0
1	I	5792	0	5623	2	0
1	J	5792	0	5623	4	0
1	W	5792	0	5623	5	0
1	X	5792	0	5623	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1122	0	1082	1	0
2	L	1122	0	1082	1	0
2	M	1122	0	1082	0	0
2	N	1122	0	1082	0	0
2	O	1122	0	1082	0	0
2	P	1122	0	1082	0	0
2	Q	1122	0	1082	0	0
2	R	1122	0	1082	1	0
2	S	1122	0	1082	0	0
2	T	1122	0	1082	2	0
2	U	1122	0	1082	2	0
2	V	1122	0	1082	0	0
3	O	5025	0	4930	2	0
3	Y	5025	0	4930	2	0
3	Z	5025	0	4930	3	0
All	All	98043	0	95250	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD21	1:A:404:MET:HE3	1.77	0.66
2:L:20:ARG:HH22	3:Z:25:ALA:H	1.55	0.54
1:J:329:LEU:HD21	1:J:404:MET:HE3	1.91	0.53
2:R:24:ARG:HH12	2:R:82:HIS:CE1	2.28	0.52
2:T:82:HIS:H	2:T:82:HIS:CD2	2.28	0.52
1:W:362:MET:HE1	1:W:373:LEU:H	1.75	0.51
1:C:41:TRP:CG	1:C:42:ASP:H	2.29	0.51
1:W:59:VAL:HG12	1:W:327:GLN:HE21	1.74	0.50
3:Y:260:THR:HG22	3:Y:261:SER:H	1.76	0.50
1:E:329:LEU:HD21	1:E:404:MET:HE3	1.94	0.49
2:U:82:HIS:CG	2:U:83:GLY:H	2.31	0.49
3:Z:203:TRP:H	3:Z:257:GLN:HE22	1.61	0.49
1:C:266:ILE:HG13	1:C:267:ALA:H	1.78	0.48
3:Y:408:ASP:H	3:Y:415:ILE:HG22	1.80	0.47
1:F:255:ILE:HD12	1:F:255:ILE:H	1.79	0.47
1:D:161:ASN:HD22	1:D:172:HIS:CD2	2.33	0.47
1:C:466:SER:H	1:C:467:ILE:HG22	1.79	0.47
1:F:272:LYS:H	1:G:134:ASP:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LYS:H	1:E:134:ASP:HB2	1.78	0.47
1:G:255:ILE:HD12	1:G:255:ILE:H	1.79	0.47
1:J:44:TRP:HE1	1:J:331:ASN:HD22	1.61	0.46
1:J:468:VAL:HA	1:J:469:ASN:HD22	1.79	0.46
1:C:255:ILE:HD12	1:C:255:ILE:H	1.81	0.46
1:D:255:ILE:H	1:D:255:ILE:HD12	1.81	0.46
3:0:407:LEU:H	3:0:407:LEU:HD23	1.80	0.46
1:I:255:ILE:HD12	1:I:255:ILE:H	1.81	0.45
1:I:41:TRP:CG	1:I:42:ASP:H	2.35	0.45
1:A:329:LEU:HD22	1:B:334:MET:HE2	1.97	0.45
2:U:74:ASN:H	2:U:75:PRO:HD2	1.82	0.45
1:C:43:ASP:H	1:C:56:GLN:HE22	1.65	0.45
1:C:329:LEU:HD21	1:C:404:MET:HE3	1.99	0.44
1:D:417:THR:HG22	1:D:419:GLY:H	1.82	0.44
1:E:255:ILE:H	1:E:255:ILE:HD12	1.82	0.44
1:H:426:ASN:H	1:H:429:GLN:HE21	1.67	0.43
2:K:74:ASN:H	2:K:75:PRO:HD2	1.83	0.43
1:W:463:ILE:HG12	1:W:464:TYR:H	1.83	0.43
1:A:37:ARG:HH22	1:A:208:VAL:HB	1.84	0.43
3:Z:340:ASN:H	3:Z:377:ASN:HD22	1.67	0.42
1:E:43:ASP:H	1:E:56:GLN:HE22	1.67	0.42
1:D:211:TRP:CD1	1:D:211:TRP:H	2.39	0.41
1:W:362:MET:HE2	1:W:362:MET:HB3	1.95	0.41
2:T:63:ILE:HD12	2:T:63:ILE:H	1.85	0.41
1:G:248:LYS:HA	1:G:511:ARG:HE	1.85	0.41
1:E:203:ASN:HA	1:E:218:GLN:HE22	1.85	0.41
1:W:496:VAL:HG13	1:W:499:LEU:HB2	2.03	0.41
1:J:255:ILE:HD12	1:J:255:ILE:H	1.86	0.40
1:B:136:SER:HB2	1:B:145:ARG:HH22	1.86	0.40
3:0:440:VAL:HG12	3:0:441:GLY:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	627/627 (100%)	625 (100%)	2 (0%)	86	86
1	B	627/627 (100%)	623 (99%)	4 (1%)	78	83
1	C	57/627 (9%)	57 (100%)	0	100	100
1	D	216/627 (34%)	215 (100%)	1 (0%)	81	83
1	E	627/627 (100%)	623 (99%)	4 (1%)	78	83
1	F	627/627 (100%)	625 (100%)	2 (0%)	86	86
1	G	627/627 (100%)	622 (99%)	5 (1%)	73	80
1	H	627/627 (100%)	625 (100%)	2 (0%)	86	86
1	I	627/627 (100%)	624 (100%)	3 (0%)	81	83
1	J	627/627 (100%)	624 (100%)	3 (0%)	81	83
1	W	627/627 (100%)	626 (100%)	1 (0%)	87	87
1	X	627/627 (100%)	625 (100%)	2 (0%)	86	86
2	K	116/116 (100%)	116 (100%)	0	100	100
2	L	116/116 (100%)	115 (99%)	1 (1%)	70	79
2	M	116/116 (100%)	116 (100%)	0	100	100
2	N	116/116 (100%)	115 (99%)	1 (1%)	70	79
2	O	116/116 (100%)	115 (99%)	1 (1%)	70	79
2	P	116/116 (100%)	116 (100%)	0	100	100
2	Q	116/116 (100%)	116 (100%)	0	100	100
2	R	116/116 (100%)	115 (99%)	1 (1%)	70	79
2	S	116/116 (100%)	116 (100%)	0	100	100
2	T	116/116 (100%)	115 (99%)	1 (1%)	70	79
2	U	116/116 (100%)	115 (99%)	1 (1%)	70	79
2	V	116/116 (100%)	116 (100%)	0	100	100
3	O	543/543 (100%)	540 (99%)	3 (1%)	78	83
3	Y	543/543 (100%)	541 (100%)	2 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Z	543/543 (100%)	543 (100%)	0	100	100
All	All	9564/10545 (91%)	9524 (100%)	40 (0%)	81	84

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	A	156	VAL
1	B	123	VAL
1	B	246	TYR
1	B	255	ILE
1	B	444	LEU
1	D	565	VAL
1	E	320	VAL
1	E	444	LEU
1	E	448	VAL
1	E	565	VAL
1	F	389	LEU
1	F	614	VAL
1	G	138	THR
1	G	156	VAL
1	G	281	ILE
1	G	320	VAL
1	G	476	ARG
1	H	157	ILE
1	H	360	GLU
1	I	150	HIS
1	I	297	HIS
1	I	708	LEU
1	J	123	VAL
1	J	469	ASN
1	J	475	PRO
2	L	123	LEU
2	N	35	THR
2	O	33	THR
2	R	123	LEU
2	T	82	HIS
2	U	82	HIS
1	W	157	ILE
1	X	248	LYS
1	X	316	TYR
3	Y	183	THR

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Mol	Chain	Res	Type
3	Y	440	VAL
3	0	430	ASP
3	0	440	VAL
3	0	493	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (322) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	31	ASN
1	A	105	ASN
1	A	142	GLN
1	A	172	HIS
1	A	337	ASN
1	A	355	GLN
1	A	380	ASN
1	A	429	GLN
1	A	465	GLN
1	A	469	ASN
1	A	491	GLN
1	A	525	GLN
1	A	590	GLN
1	A	612	GLN
1	A	617	GLN
1	A	619	GLN
1	A	677	GLN
1	A	700	GLN
1	A	706	ASN
1	A	709	GLN
1	B	47	GLN
1	B	52	GLN
1	B	150	HIS
1	B	172	HIS
1	B	181	GLN
1	B	218	GLN
1	B	297	HIS
1	B	327	GLN
1	B	355	GLN
1	B	375	ASN
1	B	394	ASN
1	B	452	ASN
1	B	529	GLN

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Mol	Chain	Res	Type
1	B	573	ASN
1	B	597	GLN
1	B	610	GLN
1	B	626	GLN
1	B	627	ASN
1	B	628	GLN
1	B	656	ASN
1	B	700	GLN
1	B	706	ASN
1	B	711	GLN
1	C	47	GLN
1	C	56	GLN
1	D	505	GLN
1	D	525	GLN
1	D	573	ASN
1	D	575	GLN
1	D	601	GLN
1	D	604	GLN
1	D	612	GLN
1	D	628	GLN
1	D	642	GLN
1	D	643	ASN
1	D	655	ASN
1	D	698	HIS
1	D	700	GLN
1	E	56	GLN
1	E	140	ASN
1	E	141	ASN
1	E	142	GLN
1	E	161	ASN
1	E	172	HIS
1	E	181	GLN
1	E	182	ASN
1	E	291	GLN
1	E	297	HIS
1	E	355	GLN
1	E	394	ASN
1	E	426	ASN
1	E	436	ASN
1	E	437	GLN
1	E	529	GLN
1	E	555	GLN

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Mol	Chain	Res	Type
1	E	573	ASN
1	E	643	ASN
1	E	686	ASN
1	F	112	ASN
1	F	142	GLN
1	F	181	GLN
1	F	202	GLN
1	F	214	GLN
1	F	270	GLN
1	F	297	HIS
1	F	337	ASN
1	F	355	GLN
1	F	429	GLN
1	F	452	ASN
1	F	469	ASN
1	F	529	GLN
1	F	612	GLN
1	F	643	ASN
1	F	706	ASN
1	F	713	GLN
1	F	725	GLN
1	G	6	ASN
1	G	74	ASN
1	G	105	ASN
1	G	150	HIS
1	G	161	ASN
1	G	172	HIS
1	G	181	GLN
1	G	182	ASN
1	G	203	ASN
1	G	205	ASN
1	G	236	GLN
1	G	337	ASN
1	G	355	GLN
1	G	375	ASN
1	G	387	GLN
1	G	633	GLN
1	G	642	GLN
1	G	676	GLN
1	G	706	ASN
1	G	711	GLN
1	G	714	ASN

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Mol	Chain	Res	Type
1	H	47	GLN
1	H	56	GLN
1	H	74	ASN
1	H	118	GLN
1	H	135	GLN
1	H	140	ASN
1	H	142	GLN
1	H	155	HIS
1	H	177	HIS
1	H	203	ASN
1	H	205	ASN
1	H	218	GLN
1	H	270	GLN
1	H	291	GLN
1	H	297	HIS
1	H	327	GLN
1	H	375	ASN
1	H	399	GLN
1	H	429	GLN
1	H	525	GLN
1	H	555	GLN
1	H	601	GLN
1	H	612	GLN
1	H	633	GLN
1	H	643	ASN
1	H	676	GLN
1	H	677	GLN
1	H	713	GLN
1	H	715	GLN
1	I	31	ASN
1	I	40	GLN
1	I	74	ASN
1	I	104	HIS
1	I	105	ASN
1	I	112	ASN
1	I	150	HIS
1	I	155	HIS
1	I	172	HIS
1	I	182	ASN
1	I	203	ASN
1	I	205	ASN
1	I	337	ASN

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Mol	Chain	Res	Type
1	I	361	HIS
1	I	375	ASN
1	I	426	ASN
1	I	436	ASN
1	I	508	ASN
1	I	655	ASN
1	I	662	GLN
1	I	700	GLN
1	I	725	GLN
1	J	31	ASN
1	J	155	HIS
1	J	172	HIS
1	J	214	GLN
1	J	270	GLN
1	J	380	ASN
1	J	429	GLN
1	J	469	ASN
1	J	505	GLN
1	J	508	ASN
1	J	529	GLN
1	J	544	GLN
1	J	555	GLN
1	J	612	GLN
1	J	627	ASN
1	J	643	ASN
1	J	646	ASN
1	J	656	ASN
1	J	676	GLN
1	J	698	HIS
1	J	700	GLN
1	J	706	ASN
1	J	725	GLN
2	K	40	GLN
2	K	58	GLN
2	K	153	ASN
2	L	43	GLN
2	L	95	ASN
2	L	153	ASN
2	M	58	GLN
2	M	82	HIS
2	M	153	ASN
2	O	40	GLN

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Mol	Chain	Res	Type
2	O	82	HIS
2	O	94	HIS
2	O	156	HIS
2	P	95	ASN
2	Q	40	GLN
2	Q	94	HIS
2	Q	151	ASN
2	Q	153	ASN
2	R	82	HIS
2	R	94	HIS
2	R	126	GLN
2	S	94	HIS
2	S	95	ASN
2	S	153	ASN
2	S	156	HIS
2	T	82	HIS
2	T	126	GLN
2	T	153	ASN
2	U	82	HIS
2	V	95	ASN
2	V	147	ASN
1	W	104	HIS
1	W	105	ASN
1	W	135	GLN
1	W	150	HIS
1	W	172	HIS
1	W	181	GLN
1	W	203	ASN
1	W	214	GLN
1	W	297	HIS
1	W	327	GLN
1	W	331	ASN
1	W	375	ASN
1	W	394	ASN
1	W	429	GLN
1	W	477	ASN
1	W	505	GLN
1	W	529	GLN
1	W	573	ASN
1	W	590	GLN
1	W	610	GLN
1	W	612	GLN

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Mol	Chain	Res	Type
1	W	686	ASN
1	W	714	ASN
1	X	31	ASN
1	X	56	GLN
1	X	104	HIS
1	X	141	ASN
1	X	142	GLN
1	X	150	HIS
1	X	177	HIS
1	X	270	GLN
1	X	291	GLN
1	X	355	GLN
1	X	429	GLN
1	X	439	ASN
1	X	452	ASN
1	X	465	GLN
1	X	529	GLN
1	X	555	GLN
1	X	617	GLN
1	X	656	ASN
1	X	709	GLN
1	X	714	ASN
3	Y	28	ASN
3	Y	99	GLN
3	Y	105	ASN
3	Y	152	ASN
3	Y	179	ASN
3	Y	298	ASN
3	Y	311	ASN
3	Y	336	GLN
3	Y	340	ASN
3	Y	381	GLN
3	Y	487	GLN
3	Y	548	ASN
3	Y	580	HIS
3	Y	610	ASN
3	Y	611	HIS
3	Y	656	ASN
3	Z	12	ASN
3	Z	53	ASN
3	Z	113	GLN
3	Z	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Z	257	GLN
3	Z	274	HIS
3	Z	289	HIS
3	Z	298	ASN
3	Z	311	ASN
3	Z	336	GLN
3	Z	340	ASN
3	Z	431	ASN
3	Z	469	HIS
3	Z	521	ASN
3	Z	540	ASN
3	Z	548	ASN
3	Z	552	ASN
3	Z	580	HIS
3	Z	593	GLN
3	Z	611	HIS
3	Z	644	ASN
3	Z	656	ASN
3	0	46	GLN
3	0	60	GLN
3	0	96	ASN
3	0	179	ASN
3	0	297	ASN
3	0	298	ASN
3	0	311	ASN
3	0	340	ASN
3	0	367	GLN
3	0	377	ASN
3	0	379	ASN
3	0	381	GLN
3	0	431	ASN
3	0	500	ASN
3	0	521	ASN
3	0	540	ASN
3	0	548	ASN
3	0	611	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

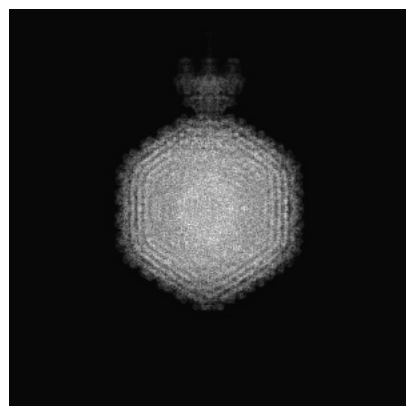
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8005. These allow visual inspection of the internal detail of the map and identification of artifacts.

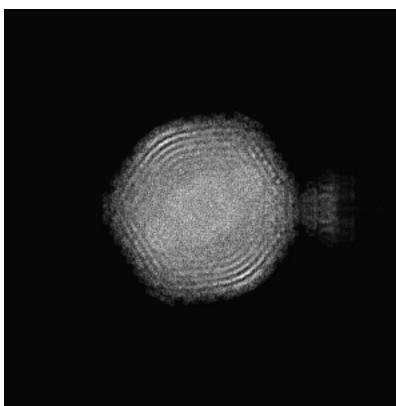
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

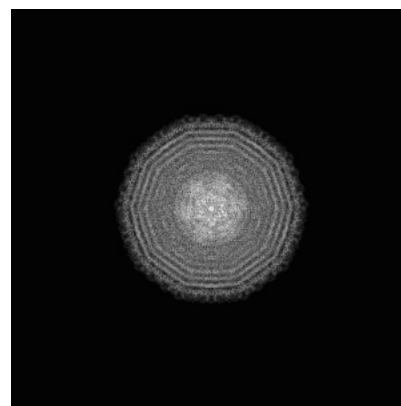
6.1.1 Primary map



X

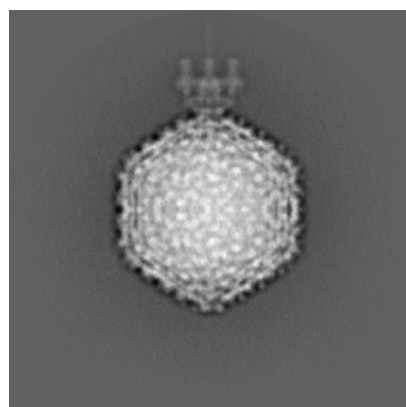


Y

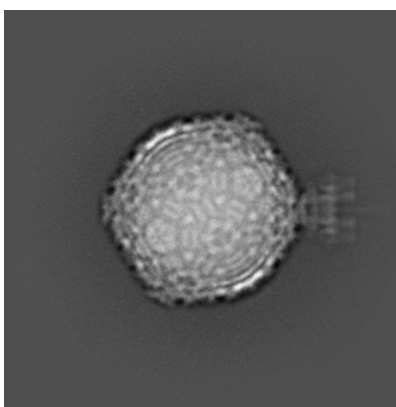


Z

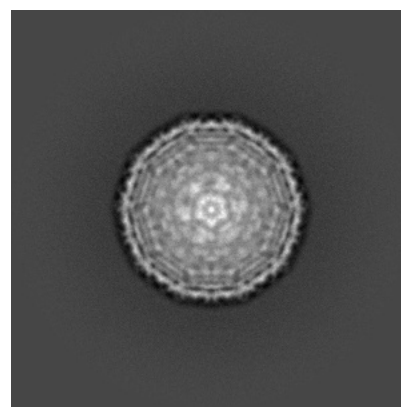
6.1.2 Raw map



X



Y

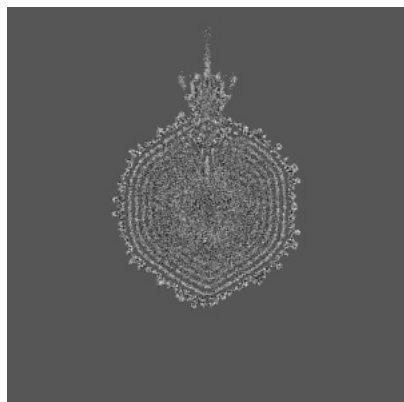


Z

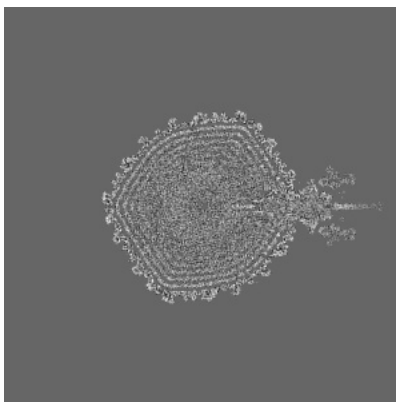
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

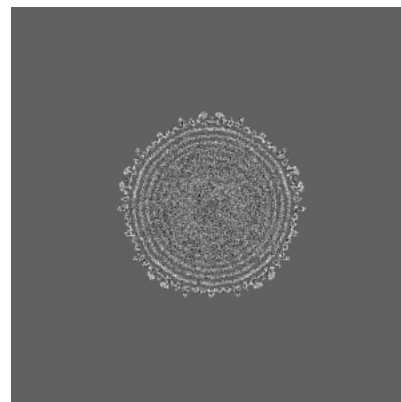
6.2.1 Primary map



X Index: 256

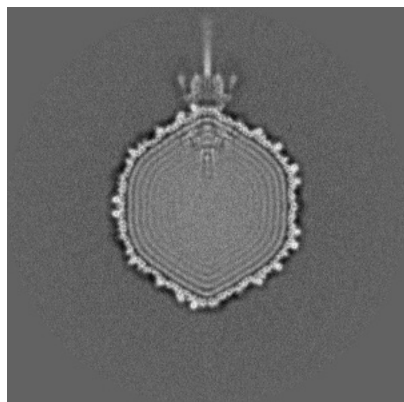


Y Index: 256

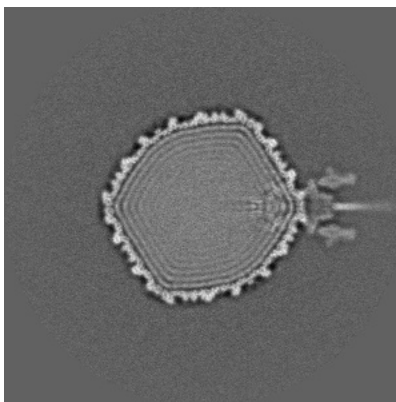


Z Index: 256

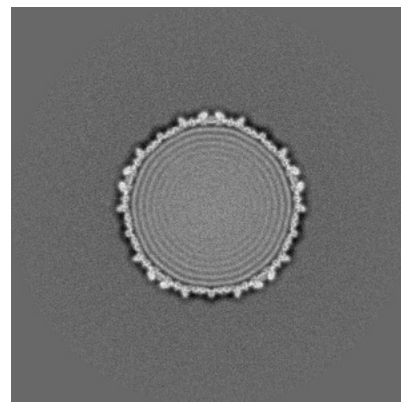
6.2.2 Raw map



X Index: 256



Y Index: 256

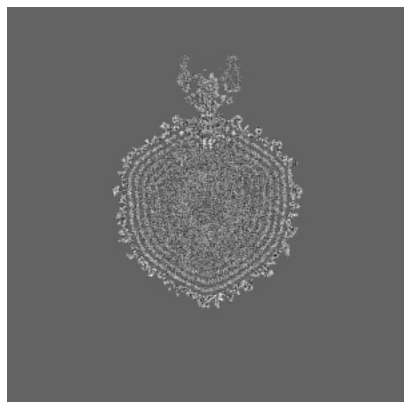


Z Index: 256

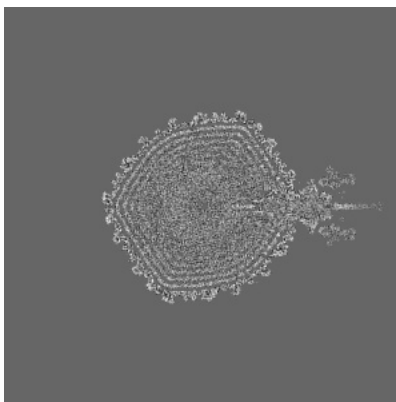
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

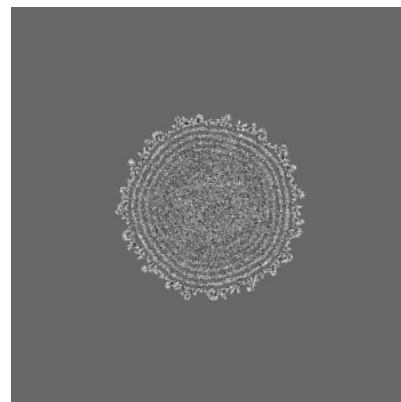
6.3.1 Primary map



X Index: 270

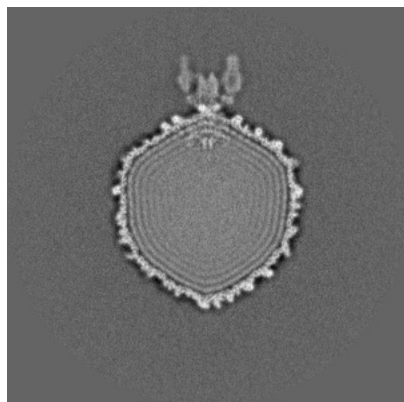


Y Index: 256

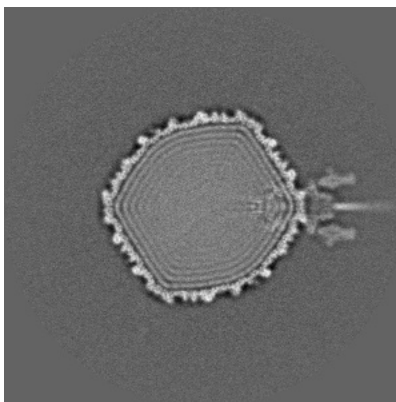


Z Index: 244

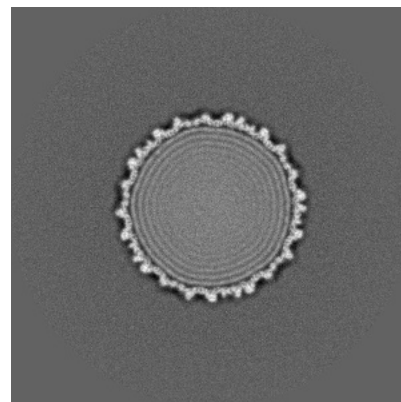
6.3.2 Raw map



X Index: 270



Y Index: 255

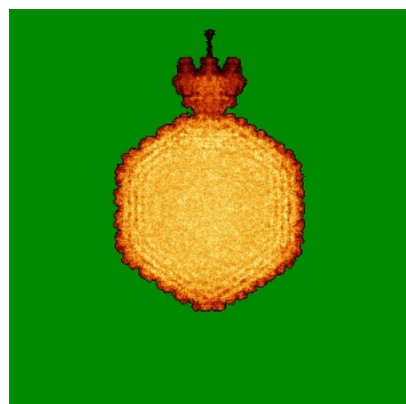


Z Index: 248

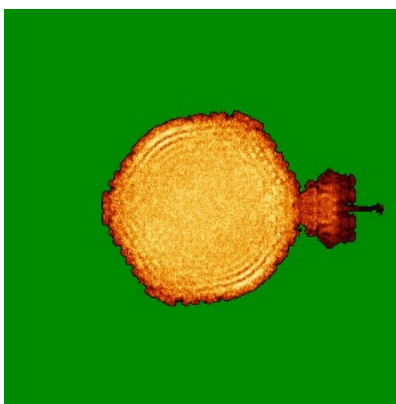
The images above show the largest variance slices of the map in three orthogonal directions.

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

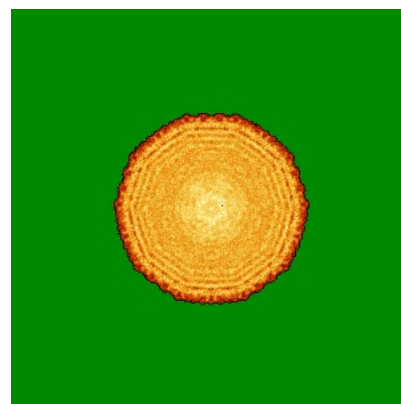
6.4.1 Primary map



X

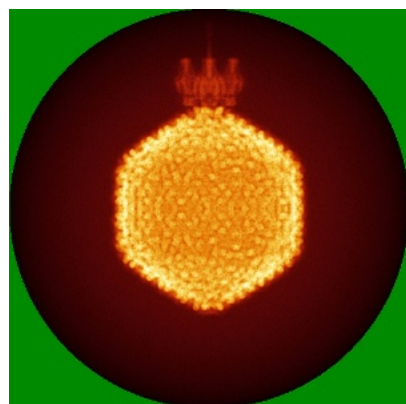


Y

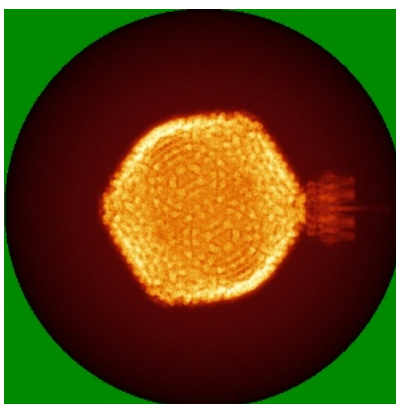


Z

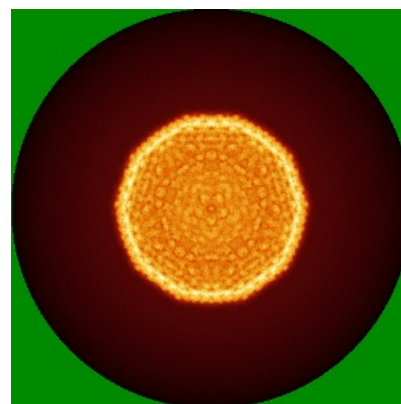
6.4.2 Raw map



X



Y

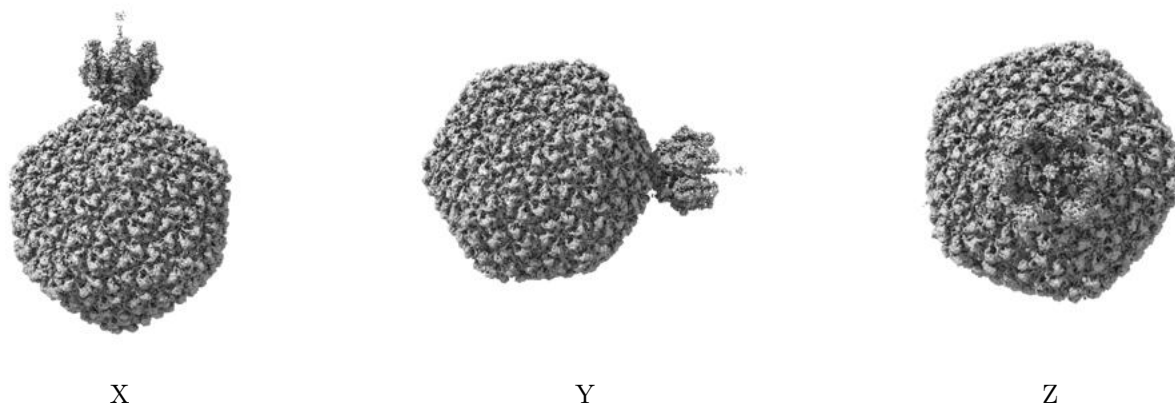


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

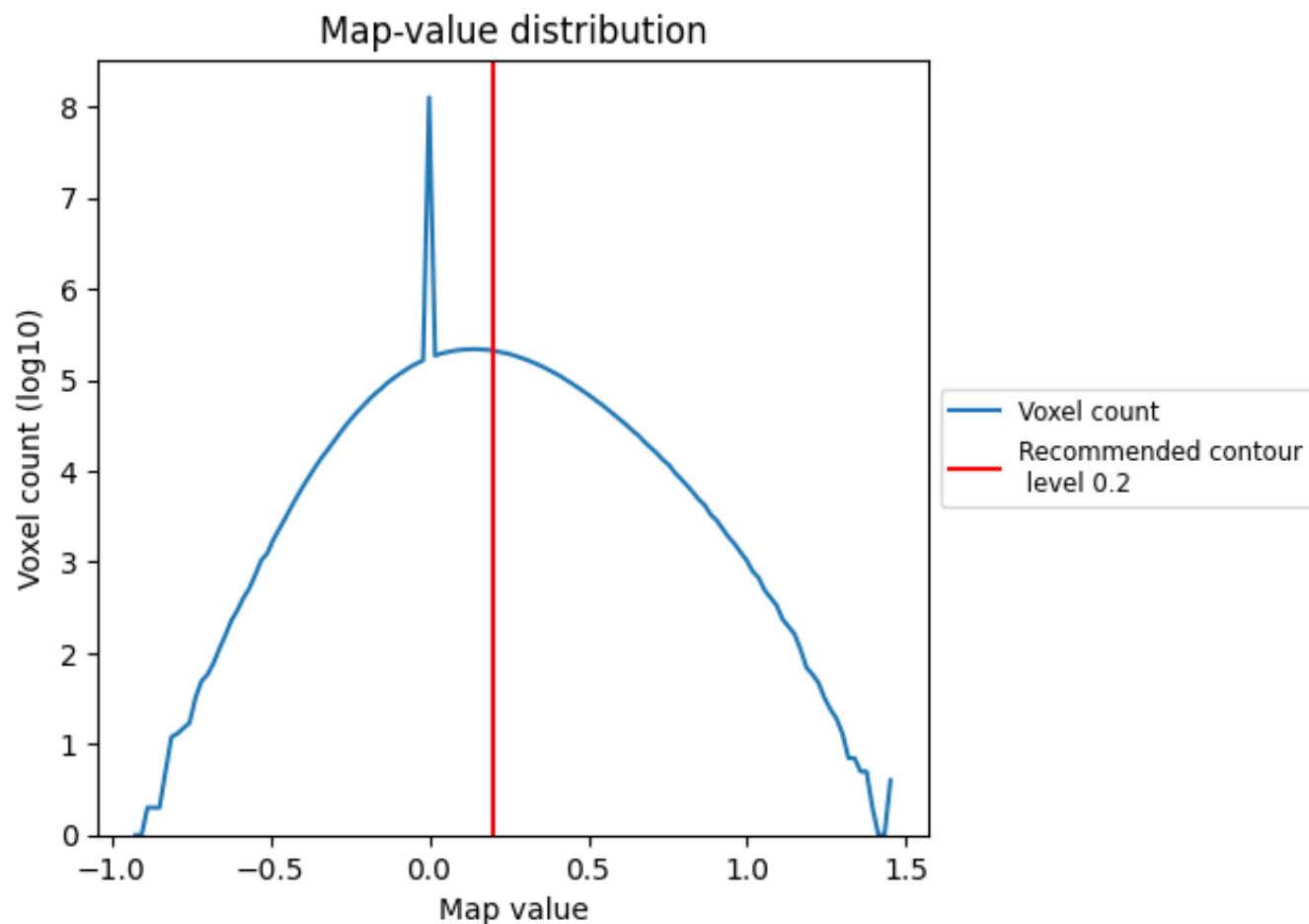
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

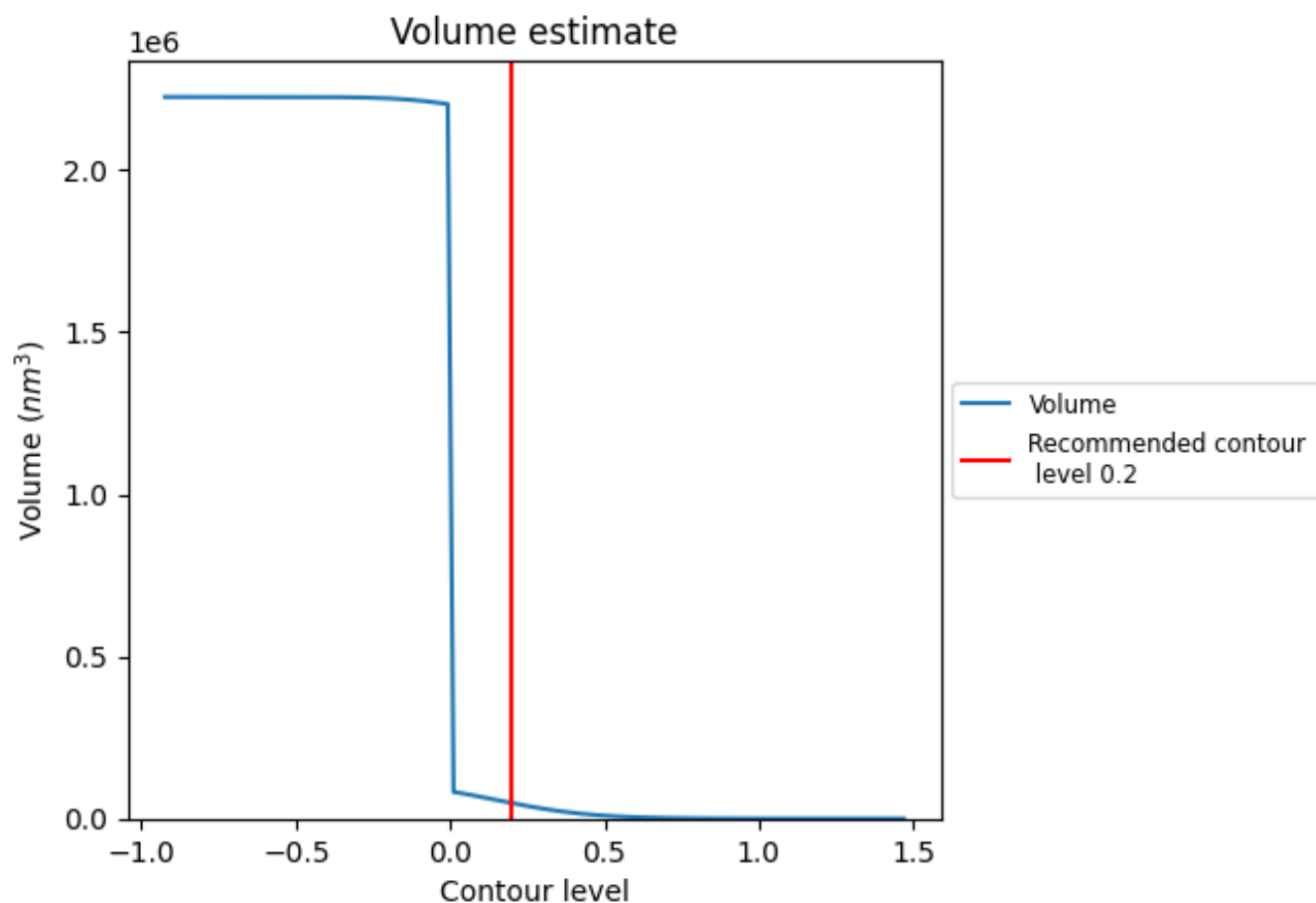
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

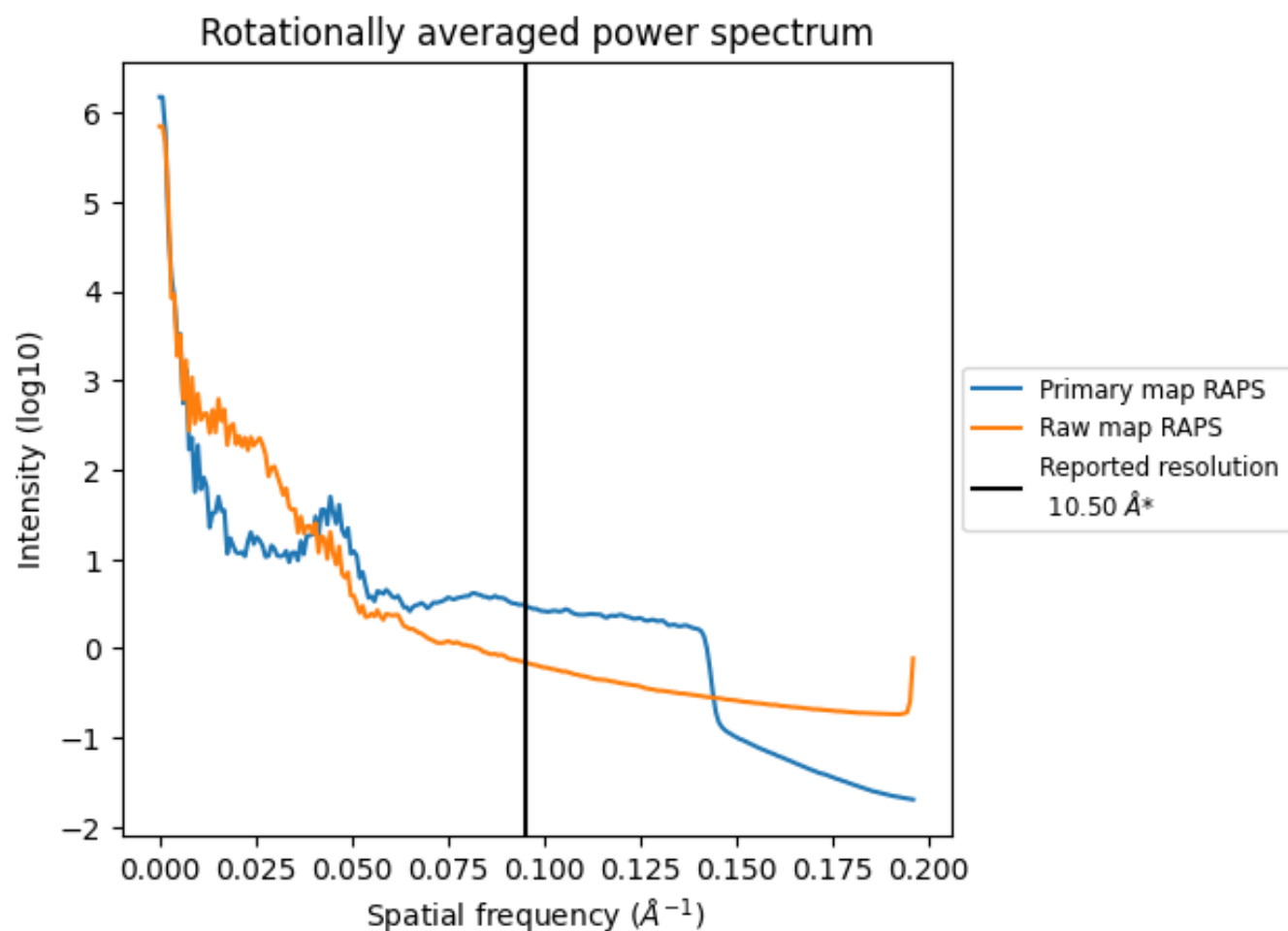
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47930 nm³; this corresponds to an approximate mass of 43297 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 ⓘ

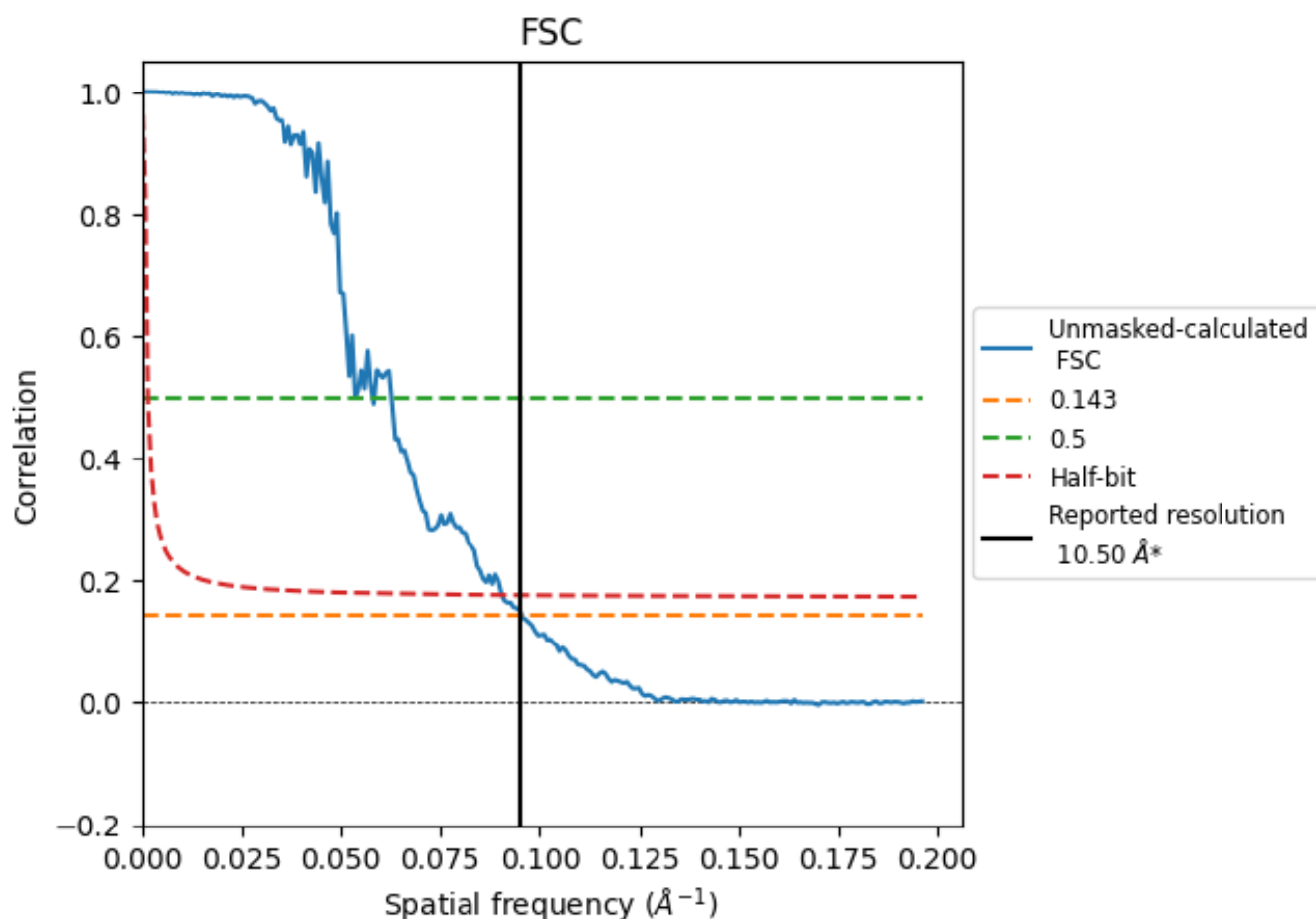


*Reported resolution corresponds to spatial frequency of 0.095 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.095 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.47	18.66	11.05

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

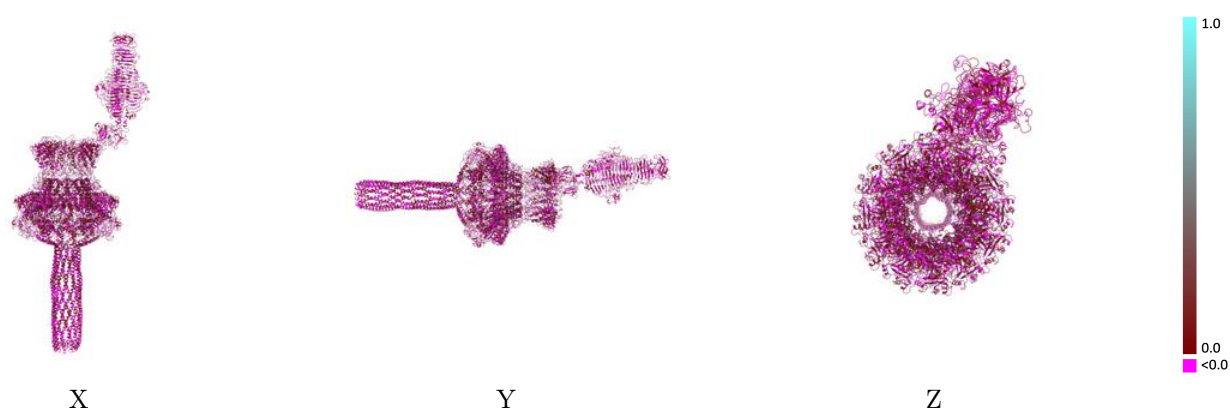
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8005 and PDB model 5GAI. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

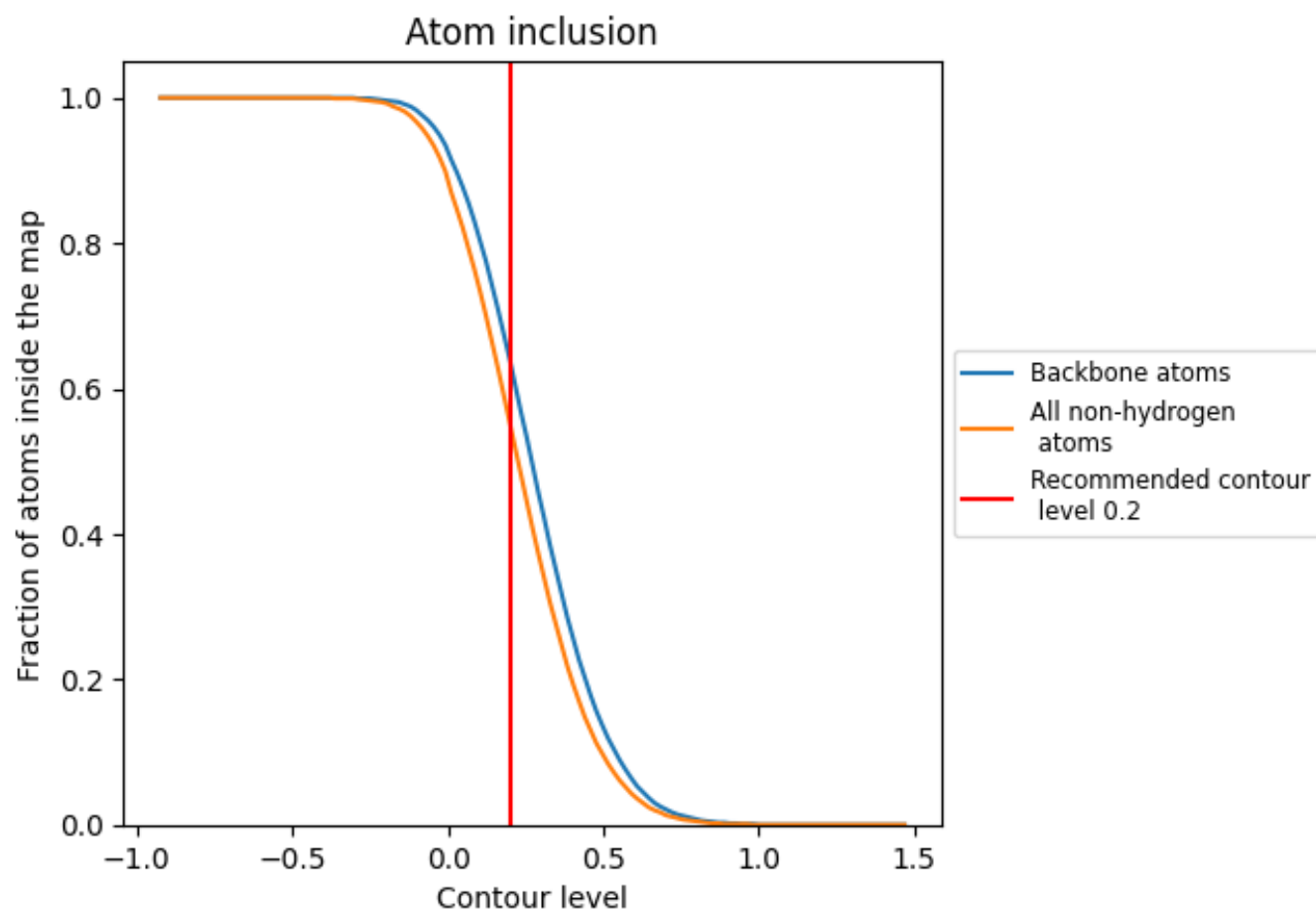


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 55% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.0410
O	 0.4460	 0.0300
A	 0.5770	 0.0430
B	 0.5640	 0.0440
C	 0.5640	 0.0370
D	 0.5780	 0.0410
E	 0.5680	 0.0420
F	 0.6000	 0.0470
G	 0.5830	 0.0480
H	 0.5700	 0.0380
I	 0.5750	 0.0380
J	 0.5600	 0.0430
K	 0.5790	 0.0550
L	 0.5900	 0.0610
M	 0.5810	 0.0590
N	 0.6000	 0.0680
O	 0.6030	 0.0530
P	 0.6070	 0.0460
Q	 0.5810	 0.0530
R	 0.5760	 0.0340
S	 0.5550	 0.0260
T	 0.5970	 0.0370
U	 0.6150	 0.0640
V	 0.6090	 0.0600
W	 0.5780	 0.0440
X	 0.5590	 0.0410
Y	 0.3680	 0.0150
Z	 0.4610	 0.0370

