



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2024 – 09:52 AM EDT

PDB ID : 8EON
EMDB ID : EMD-28405
Title : Pseudomonas phage E217 baseplate complex
Authors : Li, F.; Cingolani, G.; Hou, C.
Deposited on : 2022-10-03
Resolution : 3.60 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

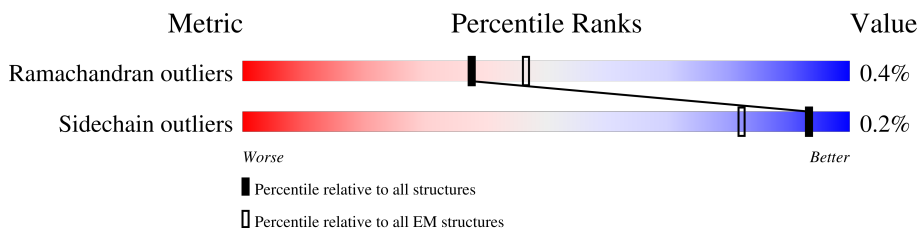
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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	G	102	17% 99% .
1	L	102	31% 99% .
1	Q	102	17% 99% .
1	V	102	32% 98% .
1	a	102	17% 99% .
1	f	102	31% 99% .
2	H	108	27% 97% .
2	M	108	21% 97% .
2	R	108	21% 98% .

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Mol	Chain	Length	Quality of chain
2	W	108	30% 98%
2	b	108	19% 98%
2	g	108	23% 98%
3	I	152	11% 99%
3	N	152	17% 99%
3	S	152	13% 99%
3	X	152	17% 99%
3	c	152	15% 99%
3	h	152	12% 99%
4	J	417	63% 100%
4	O	417	66% 100%
4	T	417	63% 100%
4	Y	417	69% 99%
4	d	417	63% 100%
4	i	417	66% 100%
4	q	417	50% 96%
4	r	417	53% 96%
4	s	417	51% 97%
4	t	417	58% 96%
4	u	417	60% 96%
4	v	417	58% 96%
5	K	500	82% 100%
5	P	500	82% 100%
5	U	500	83% 100%
5	Z	500	85% 99%

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Mol	Chain	Length	Quality of chain
5	e	500	82% 100%
5	j	500	85% 100%
6	A	172	14% 98%
6	B	172	16% 99%
6	C	172	13% 99%
7	D	193	23% 99%
7	k	193	22% 99%
7	o	193	22% 98%
8	E	287	13% 99%
8	l	287	12% 99%
8	m	287	11% 99%
9	F	219	16% 100%
9	n	219	16% 100%
9	p	219	15% 100%

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 95688 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 Baseplate component gp33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	102	816	525	136	150	5	0	0
1	L	102	816	525	136	150	5	0	0
1	Q	102	816	525	136	150	5	0	0
1	V	102	816	525	136	150	5	0	0
1	a	102	816	525	136	150	5	0	0
1	f	102	816	525	136	150	5	0	0

- Molecule 2 is a protein called Baseplate component gp34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	108	823	510	137	172	4	0	0
2	M	108	823	510	137	172	4	0	0
2	R	108	823	510	137	172	4	0	0
2	W	108	823	510	137	172	4	0	0
2	b	108	823	510	137	172	4	0	0
2	g	108	823	510	137	172	4	0	0

- Molecule 3 is a protein called Baseplate component gp36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	152	1133	726	182	221	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	S	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	X	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	c	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	h	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		

- Molecule 4 is a protein called Triplex gp44-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	O	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	T	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	Y	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	d	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	i	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	q	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	r	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	s	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	t	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	u	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	v	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		

- Molecule 5 is a protein called Triplex gp45.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	P	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	U	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	Z	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	e	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	j	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		

- Molecule 6 is a protein called Baseplate component gp37.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	172	Total	C	N	O	S	0	0
			1329	828	231	258	12		
6	B	172	Total	C	N	O	S	0	0
			1329	828	231	258	12		
6	C	172	Total	C	N	O	S	0	0
			1329	828	231	258	12		

- Molecule 7 is a protein called Baseplate component gp38.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	193	Total	C	N	O	S	0	0
			1482	937	240	298	7		
7	k	193	Total	C	N	O	S	0	0
			1482	937	240	298	7		
7	o	193	Total	C	N	O	S	0	0
			1482	937	240	298	7		

- Molecule 8 is a protein called Baseplate hub gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	287	Total	C	N	O	S	0	0
			2278	1441	398	425	14		
8	l	287	Total	C	N	O	S	0	0
			2278	1441	398	425	14		
8	m	287	Total	C	N	O	S	0	0
			2278	1441	398	425	14		

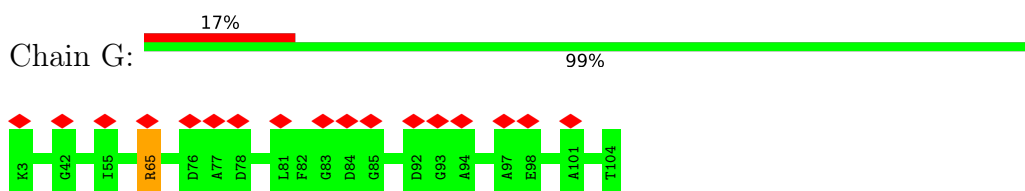
- Molecule 9 is a protein called Baseplate spike gp43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	219	Total 1687	C 1049	N 308	O 325	S 5	0	0
9	n	219	Total 1687	C 1049	N 308	O 325	S 5	0	0
9	p	219	Total 1687	C 1049	N 308	O 325	S 5	0	0

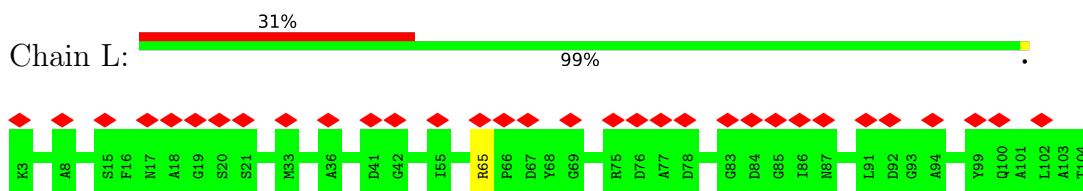
3 Residue-property plots [i](#)

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

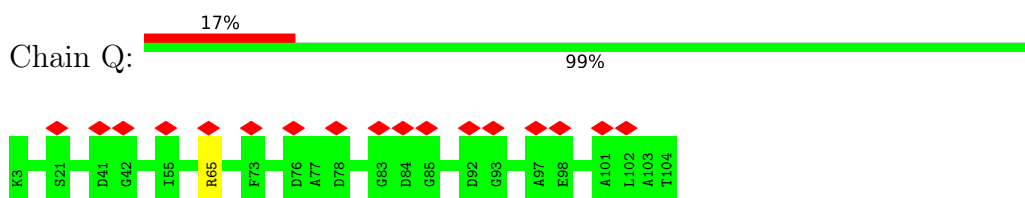
- Molecule 1: Baseplate component gp33



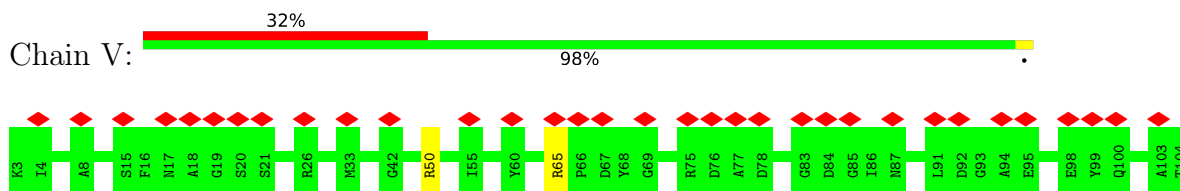
- Molecule 1: Baseplate component gp33



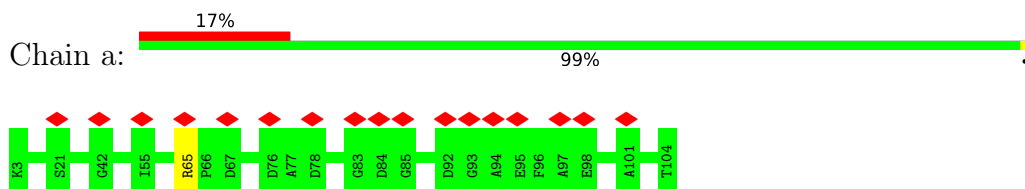
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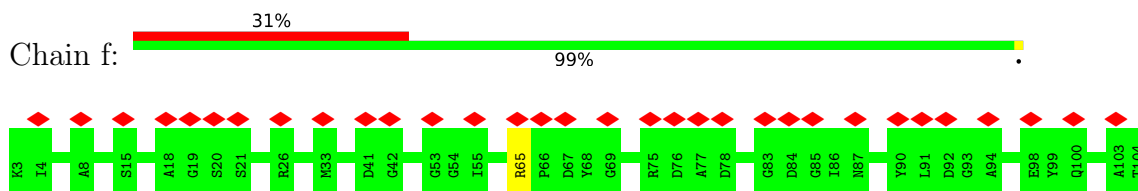
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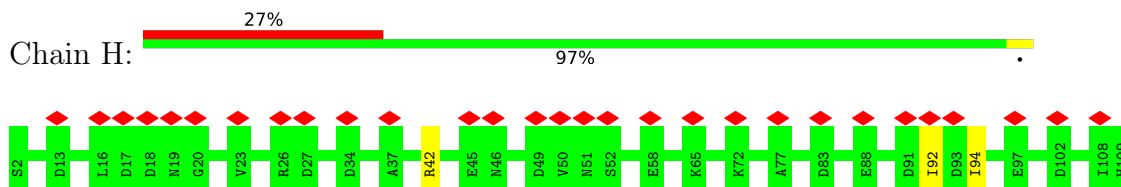
- Molecule 1: Baseplate component gp33



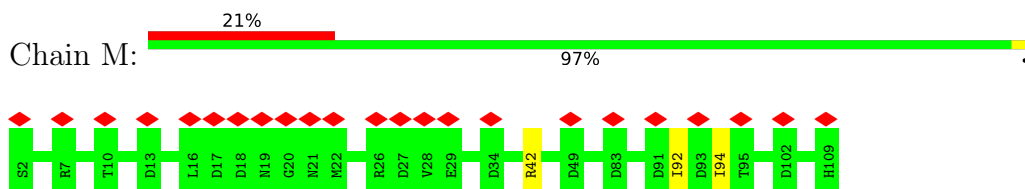
- Molecule 1: Baseplate component gp33



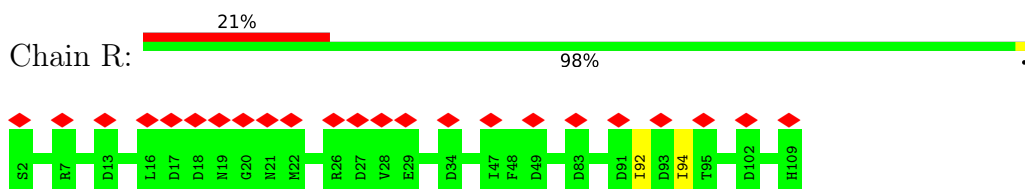
- Molecule 2: Baseplate component gp34



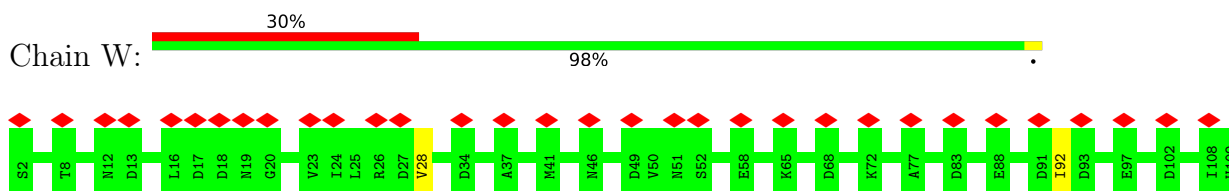
- Molecule 2: Baseplate component gp34



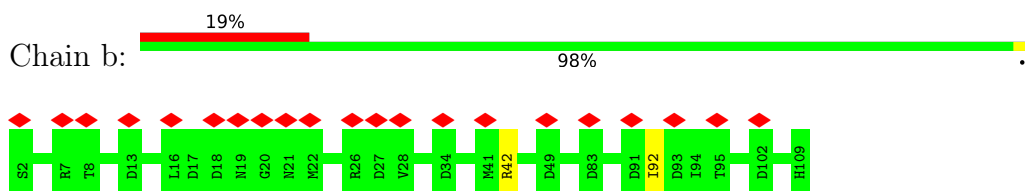
- Molecule 2: Baseplate component gp34



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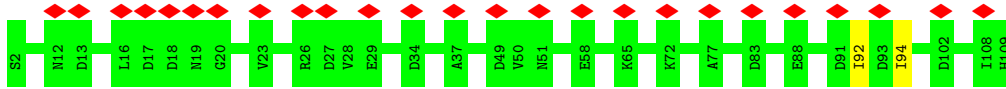


- Molecule 2: Baseplate component gp34

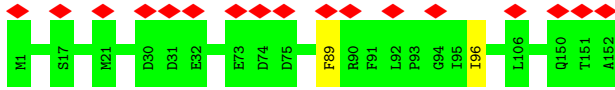


- Molecule 2: Baseplate component gp34

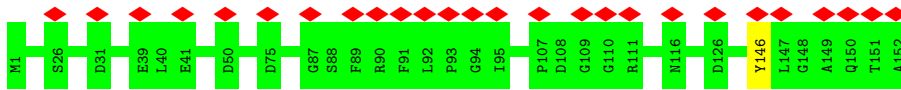




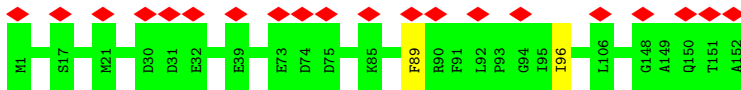
- Molecule 3: Baseplate component gp36



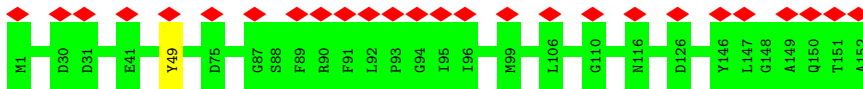
- Molecule 3: Baseplate component gp36



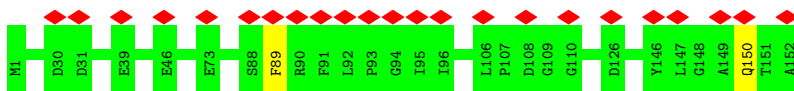
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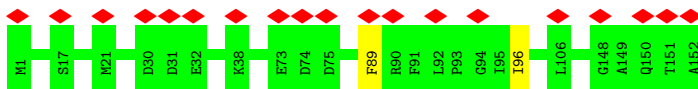
- Molecule 3: Baseplate component gp36



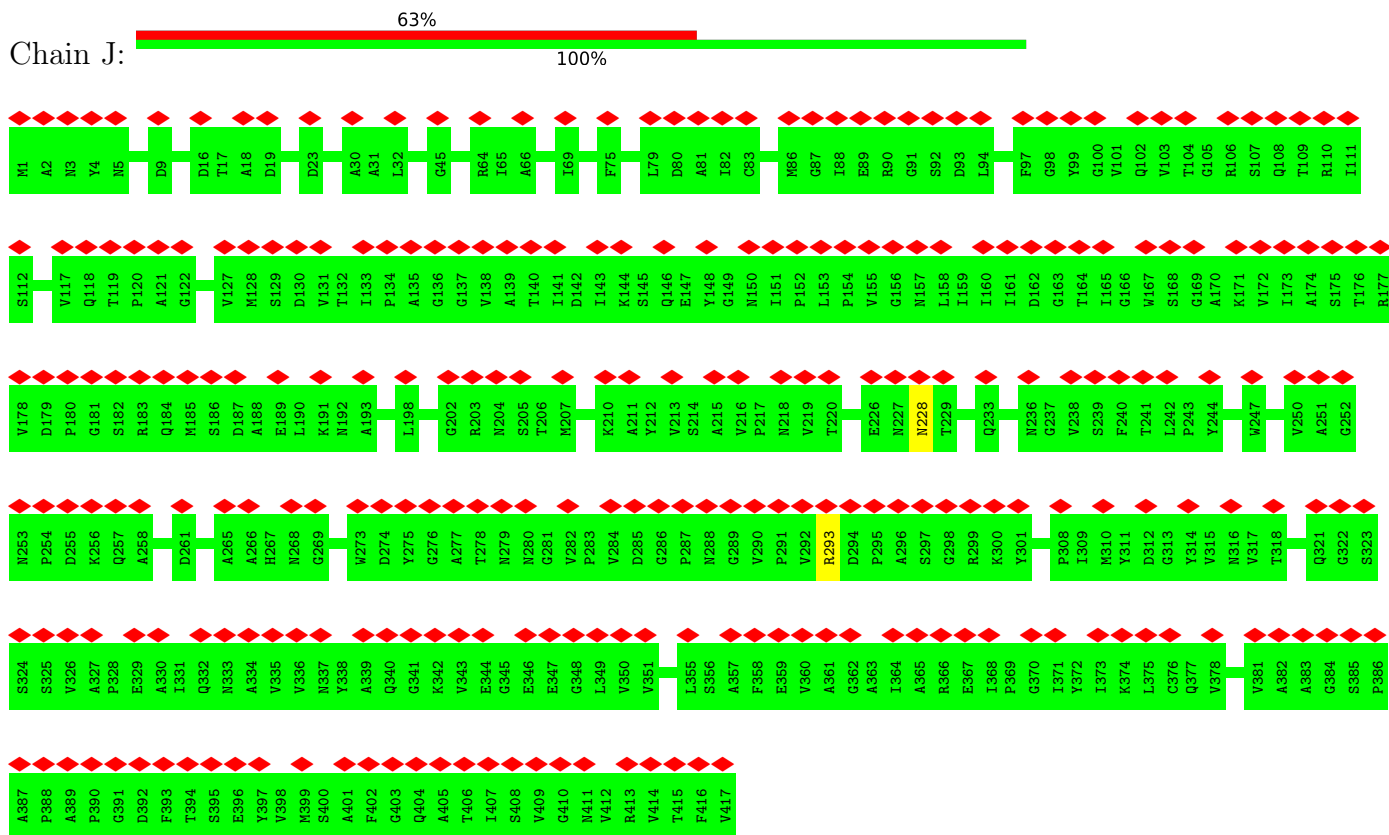
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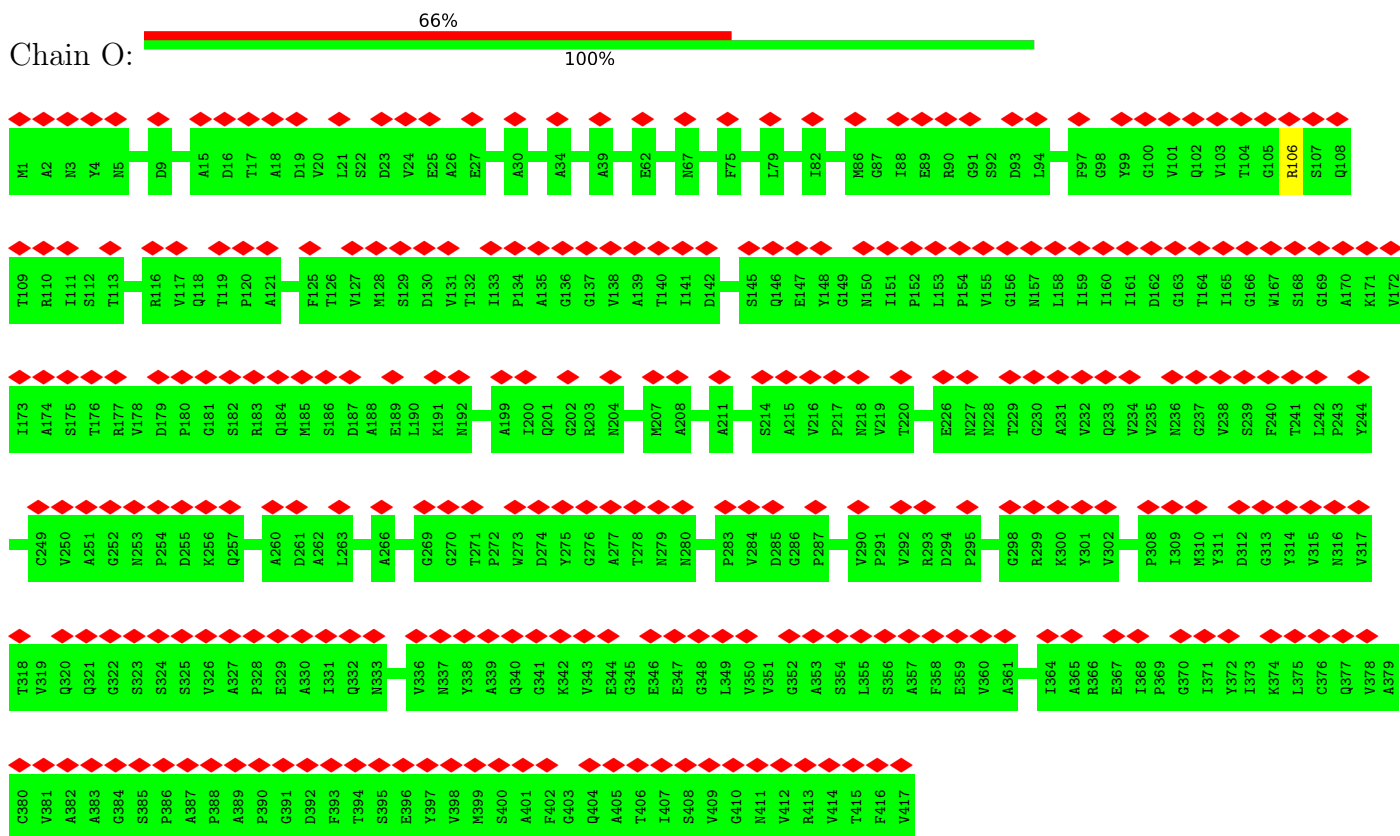
- Molecule 3: Baseplate component gp36



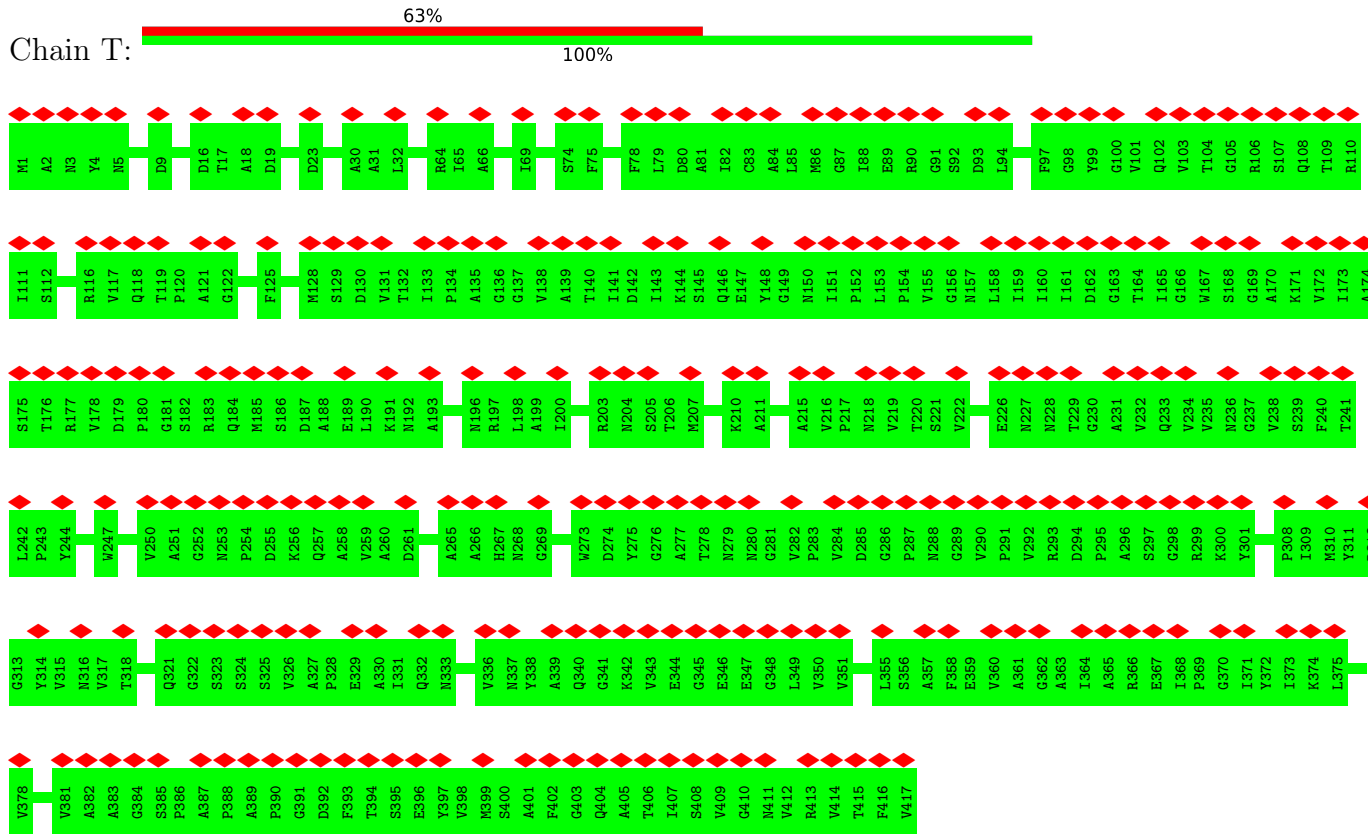
- Molecule 4: Triplex gp44-b



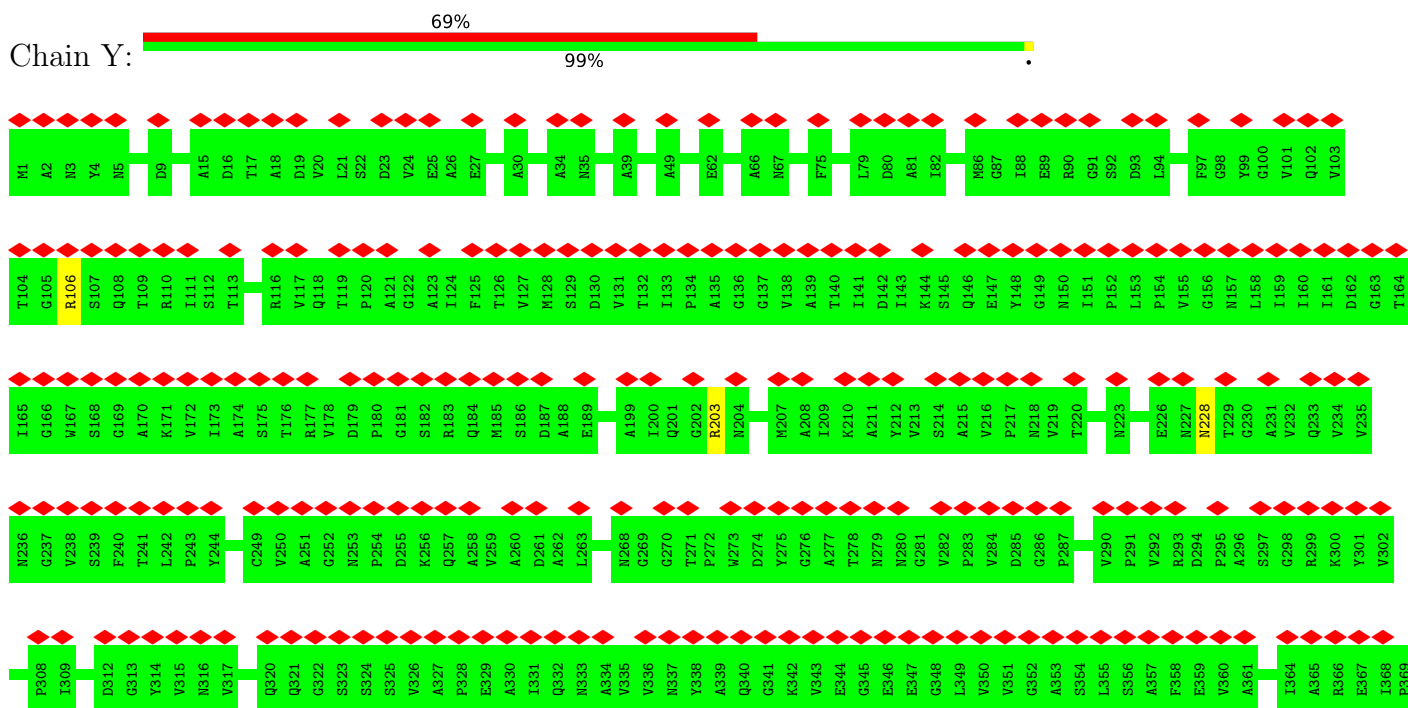
• Molecule 4: Triplex gp44-b

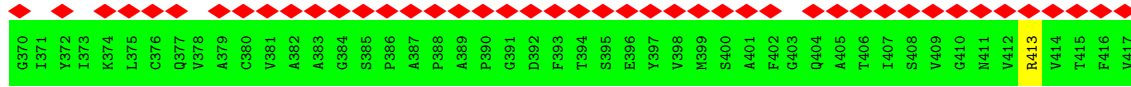


• Molecule 4: Triplex gp44-b

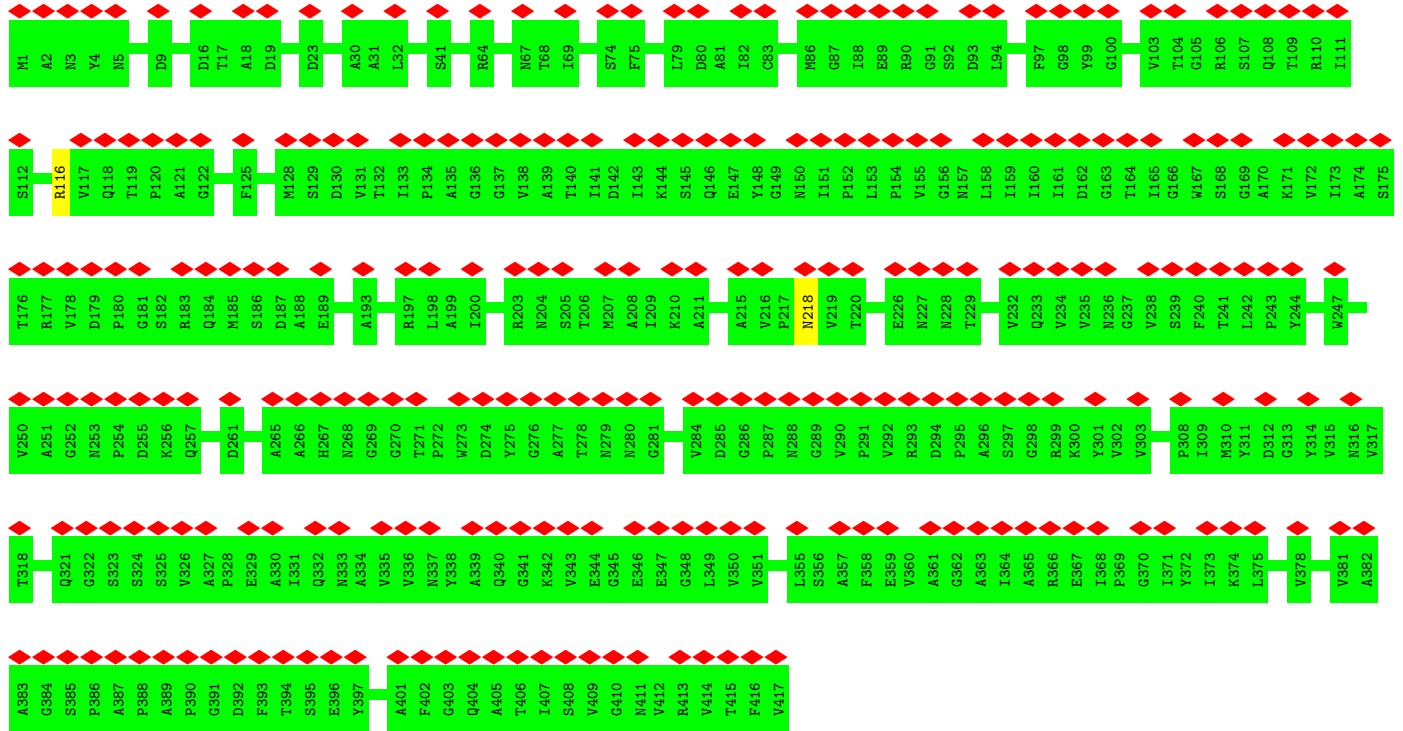


• Molecule 4: Triplex gp44-b

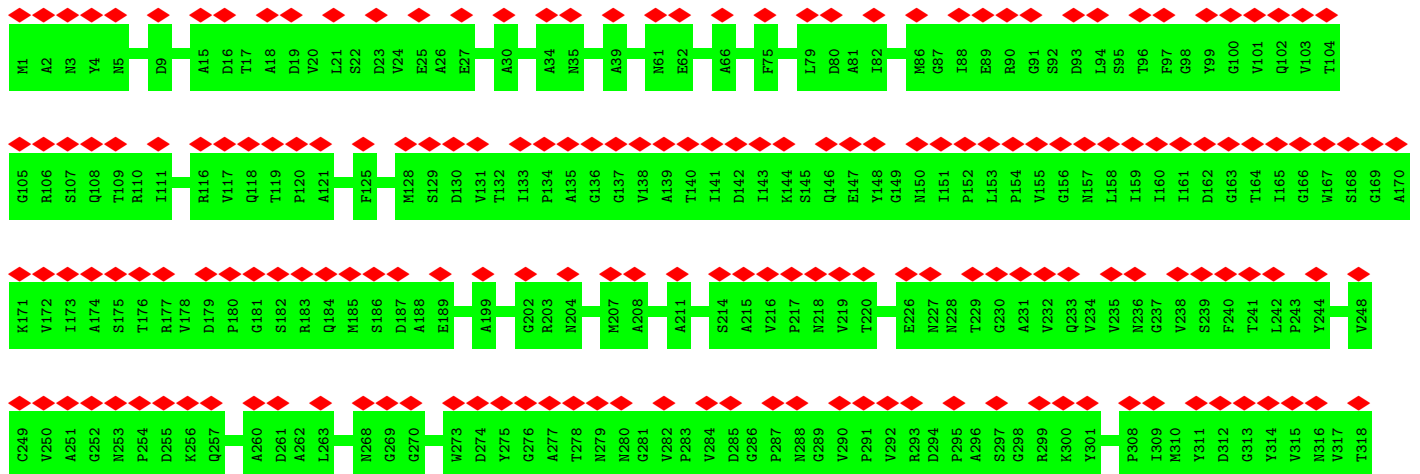




• Molecule 4: Triplex gp44-b



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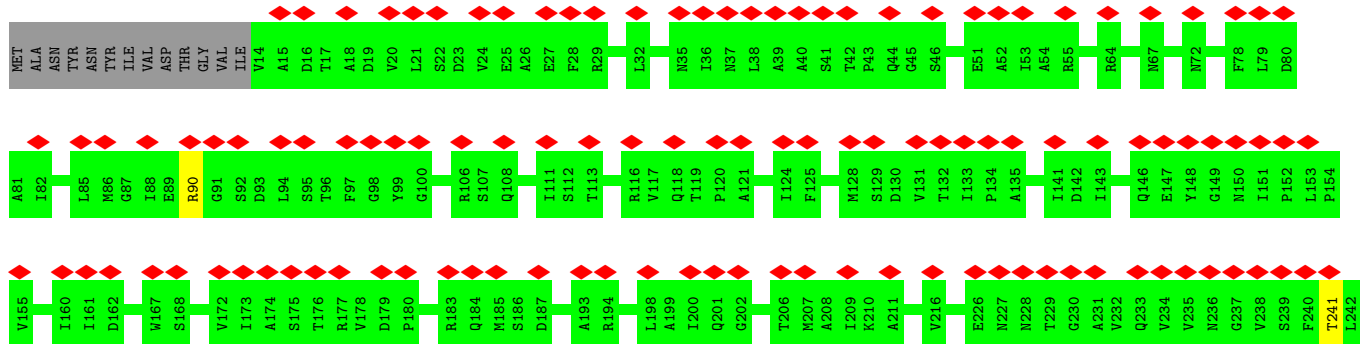


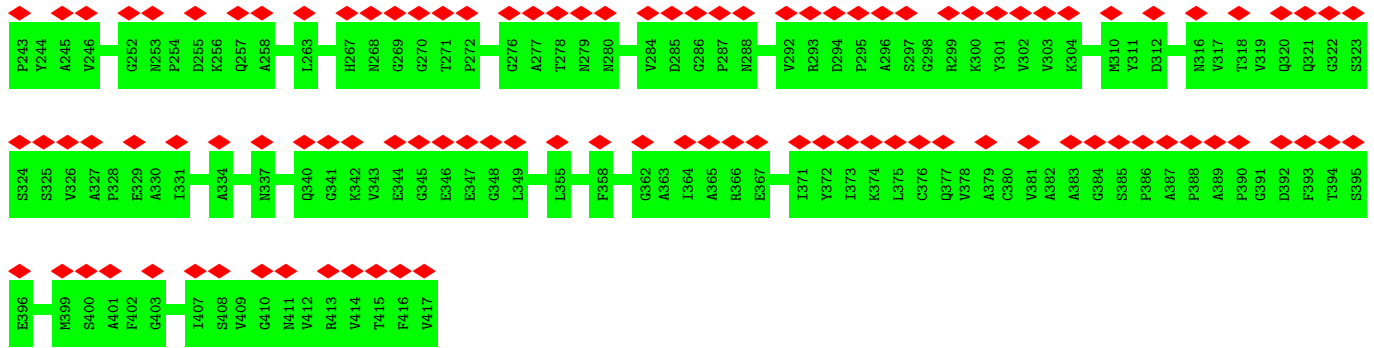


• Molecule 4: Triplex gp44-b

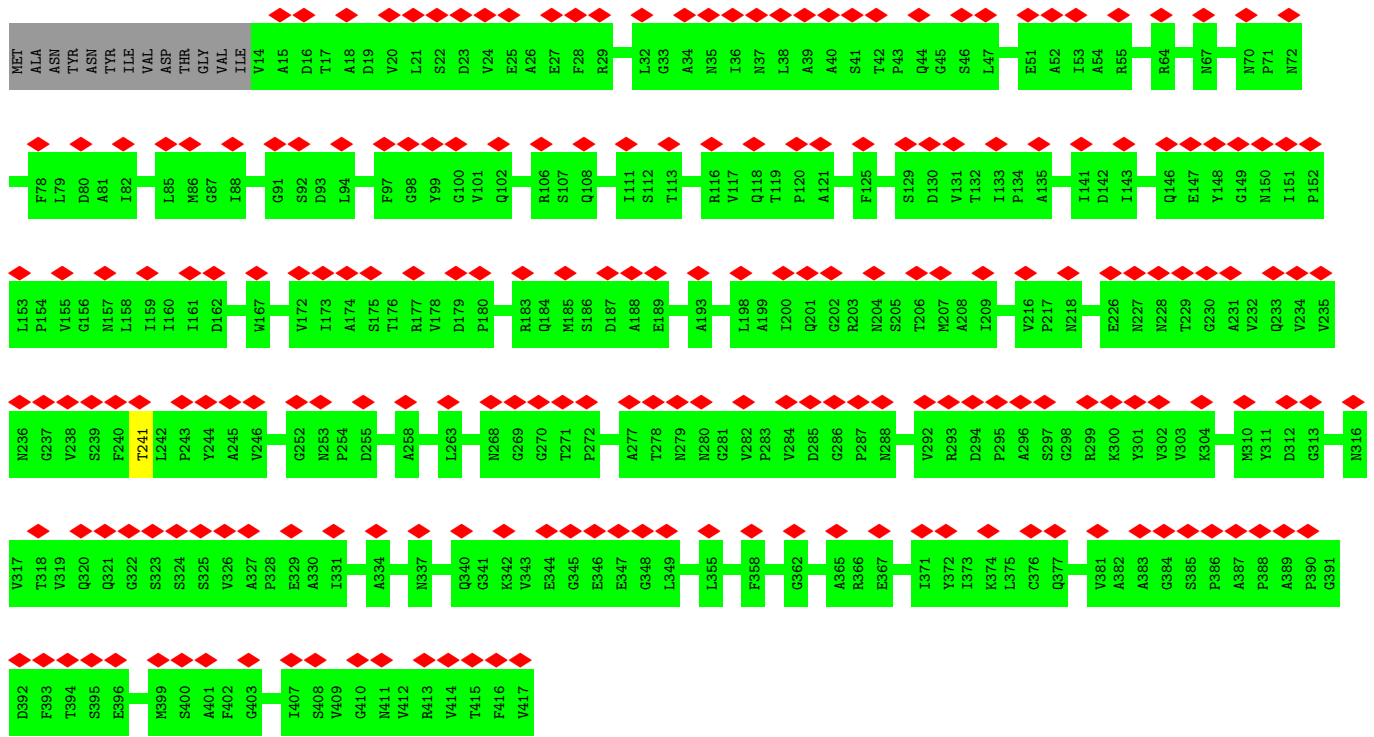


• Molecule 4: Triplex gp44-b

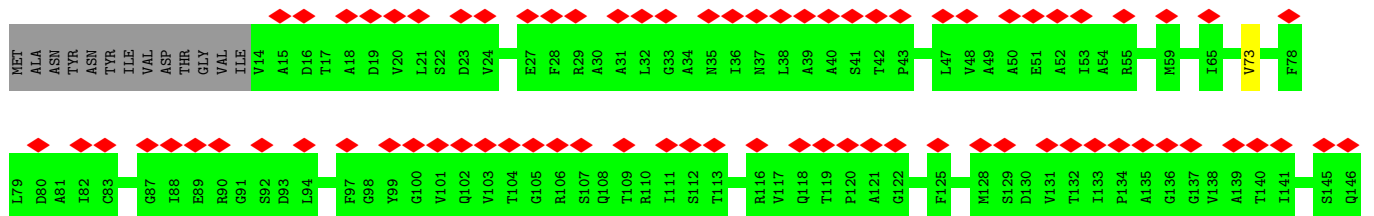
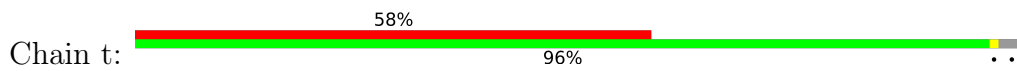


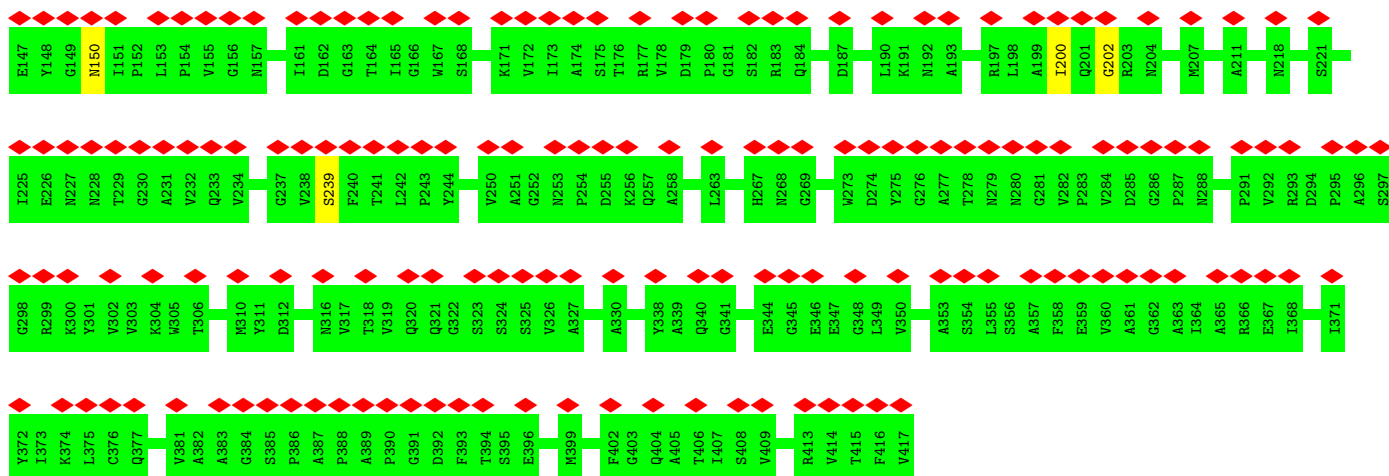


• Molecule 4: Triplex gp44-b



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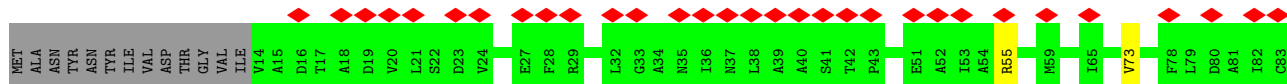
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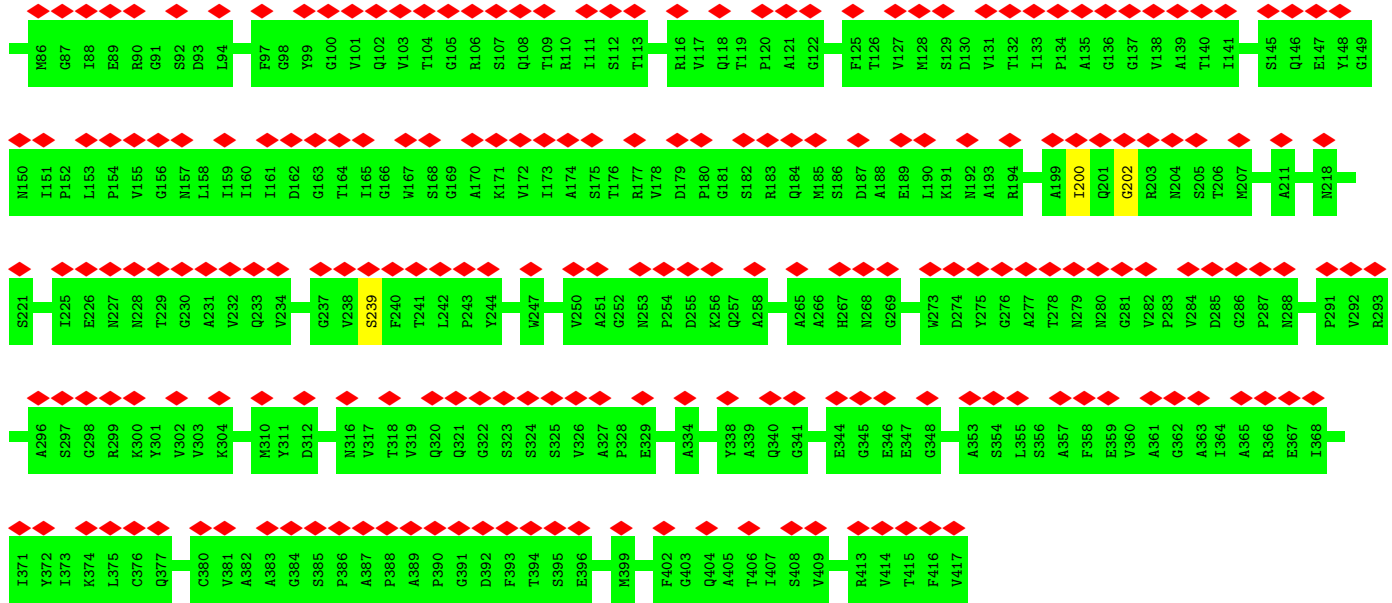
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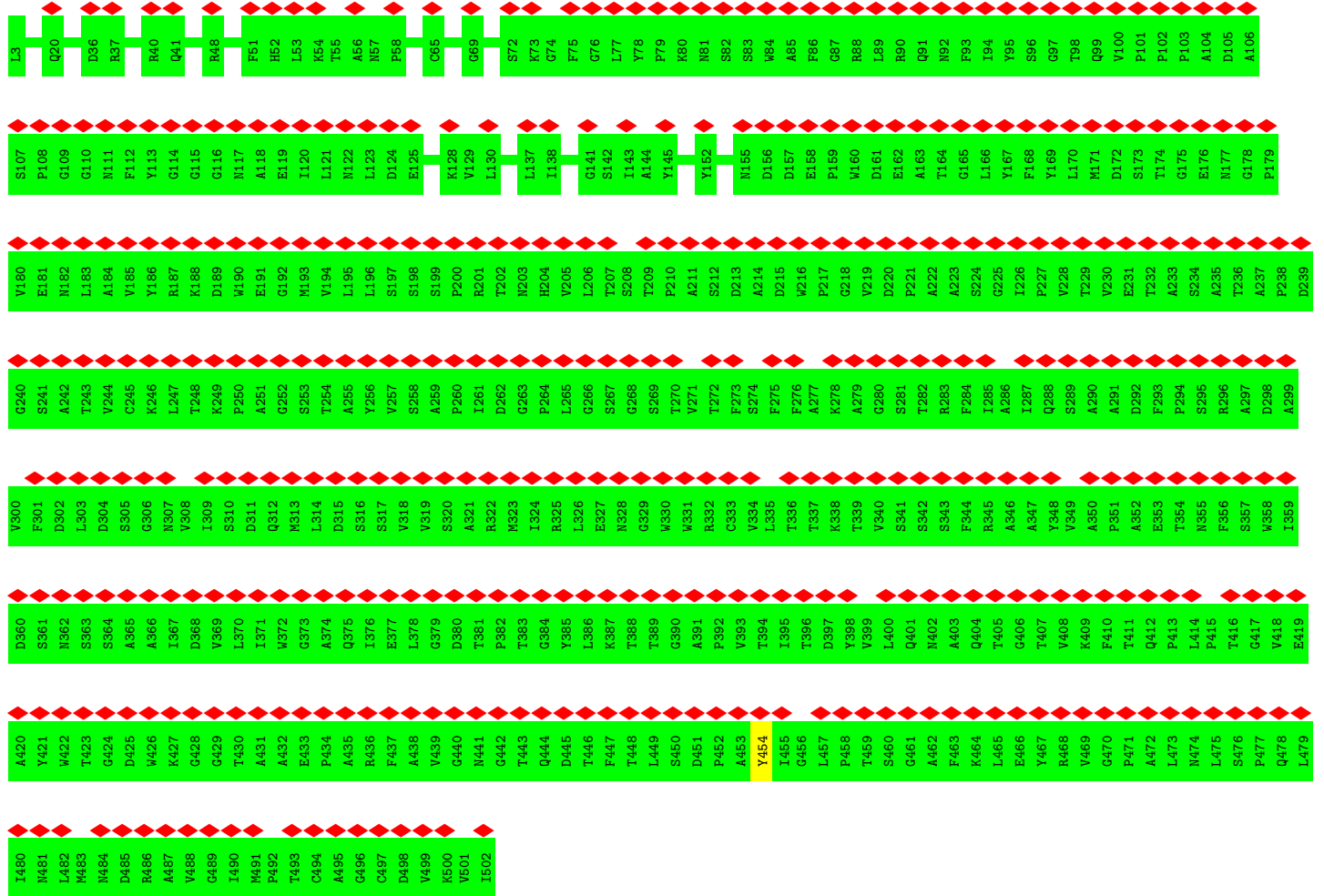
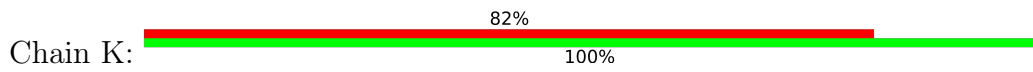
• Molecule 4: Triplex gp44-b

Chain v:

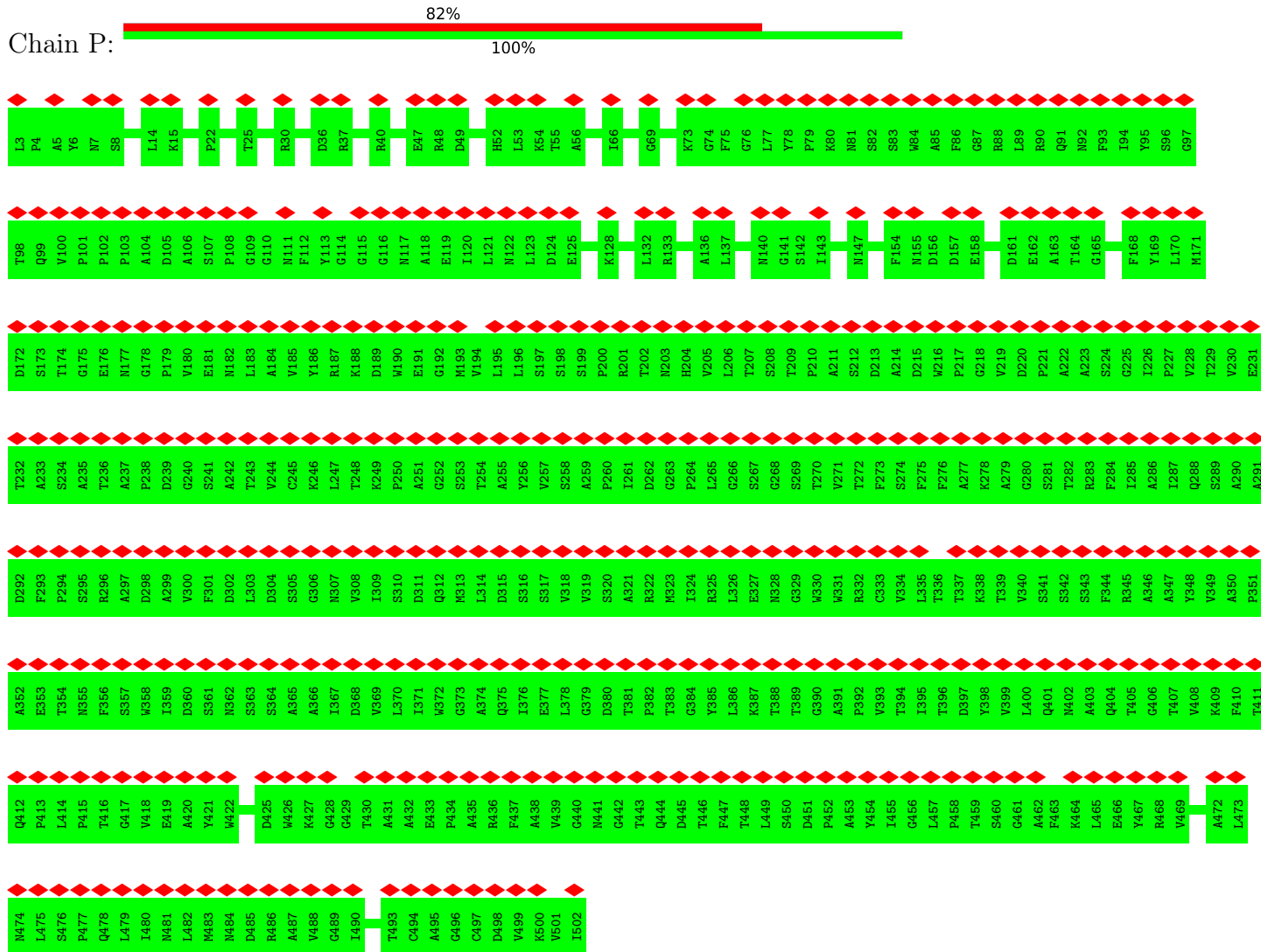




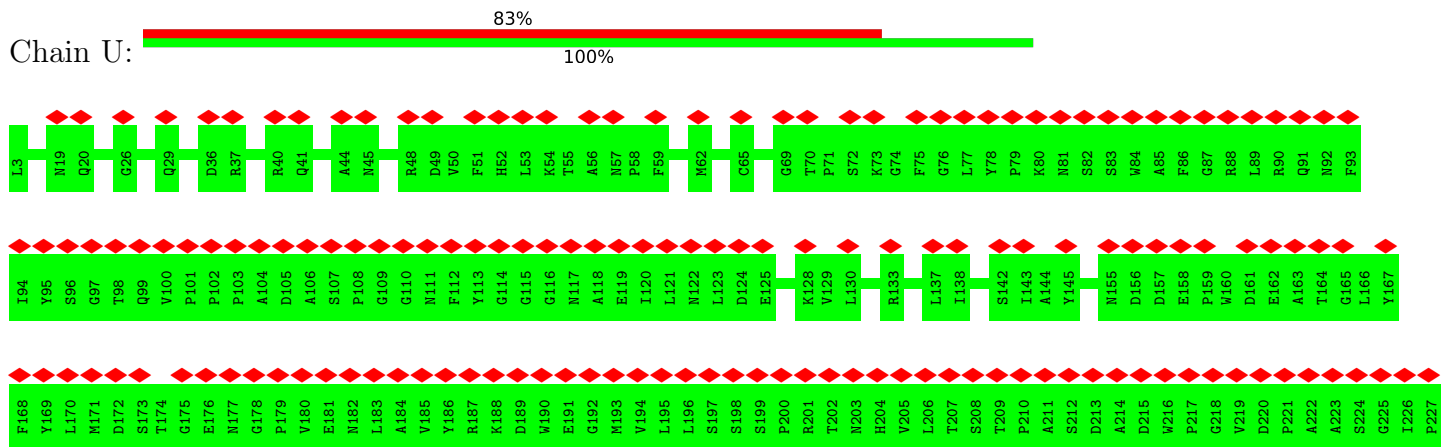
• Molecule 5: Triplex gp45



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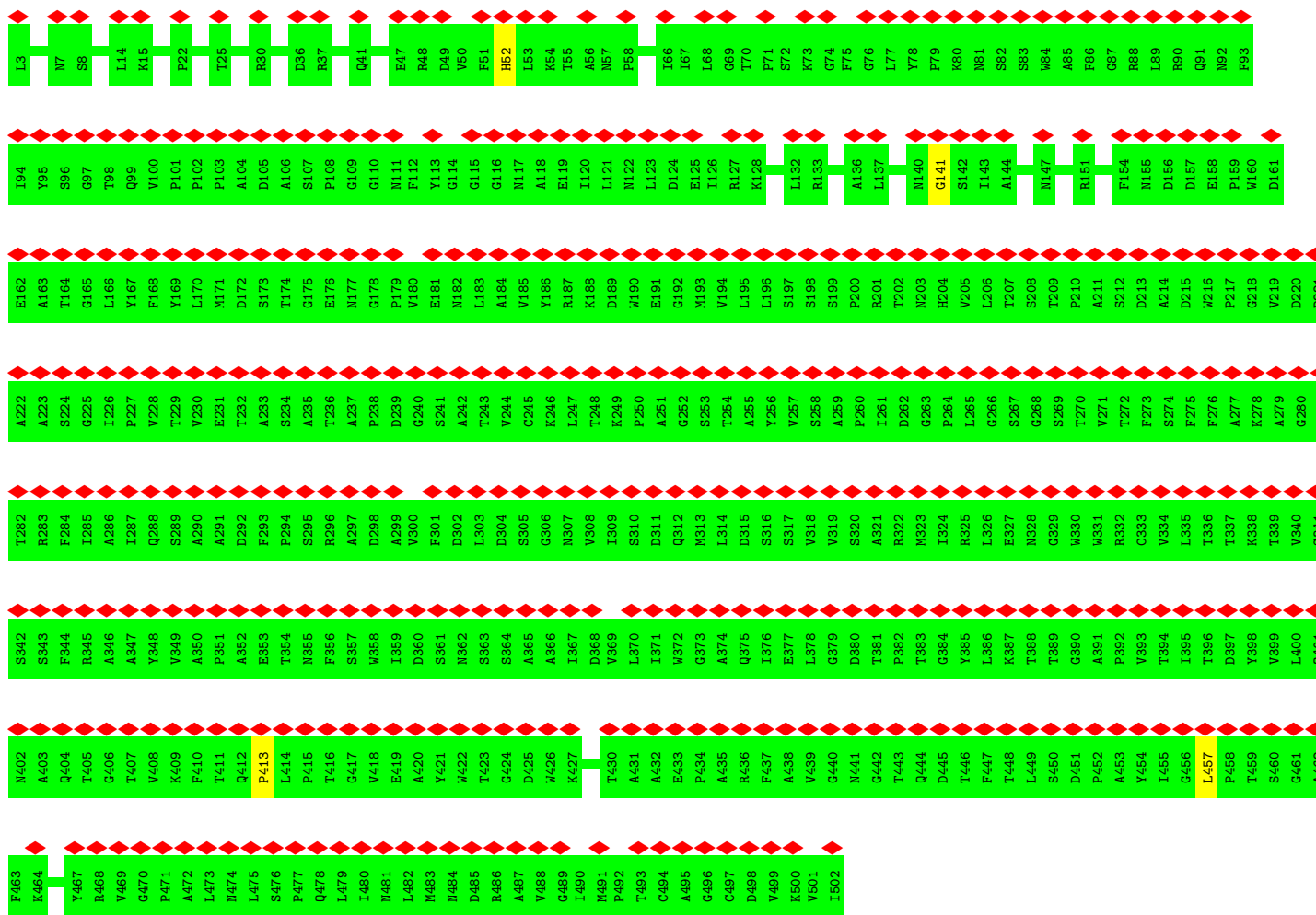


• Molecule 5: Triplex gp45

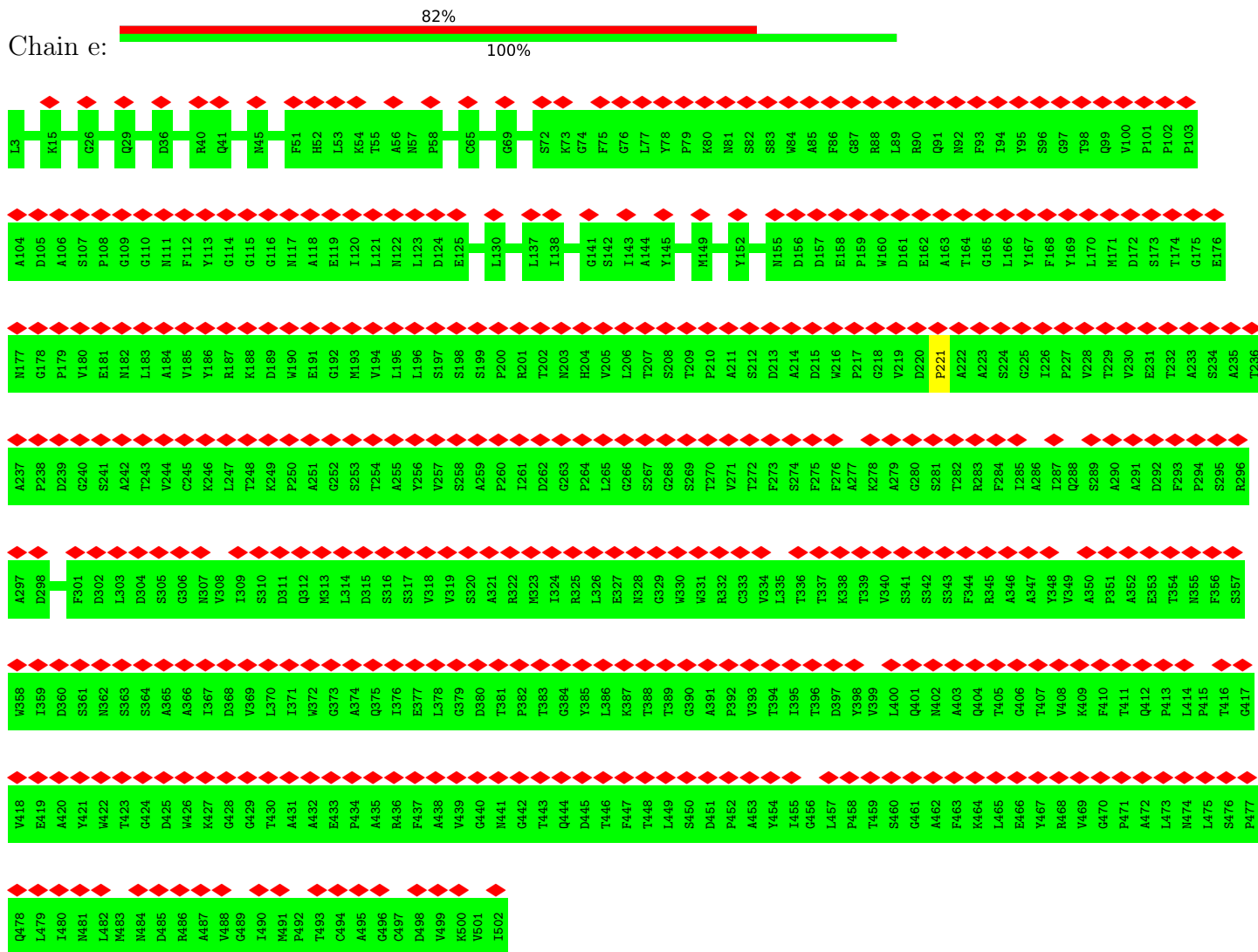




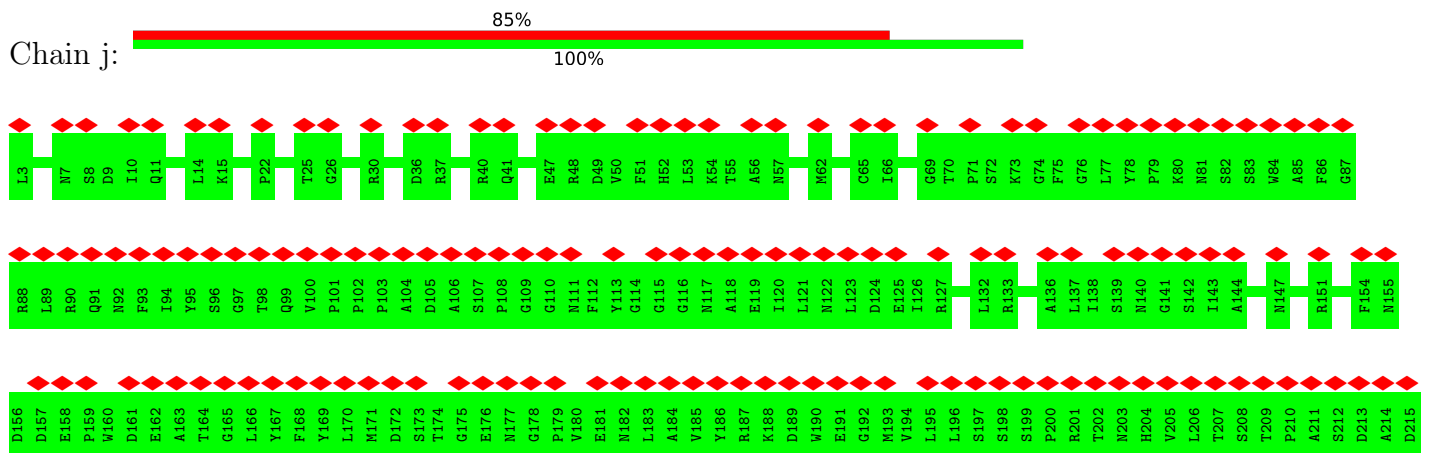
• Molecule 5: Triplex gp45

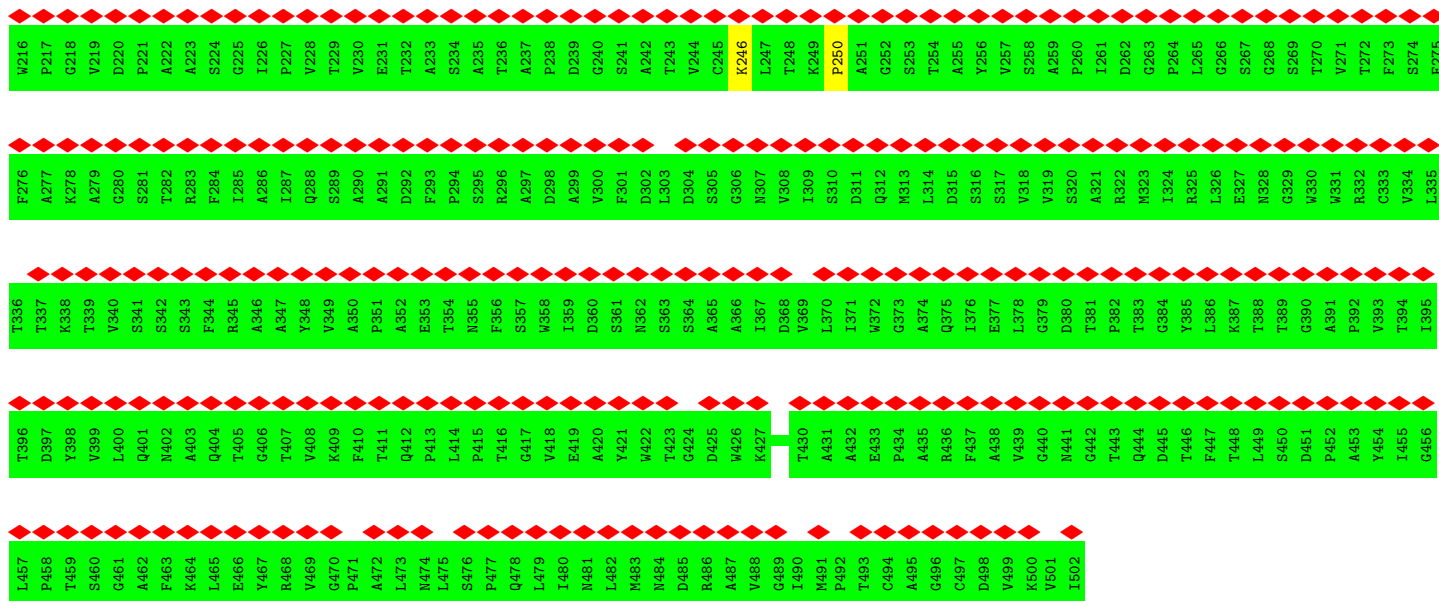


• Molecule 5: Triplex gp45

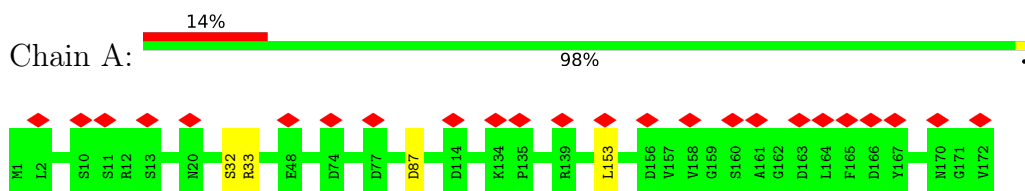


• Molecule 5: Triplex gp45

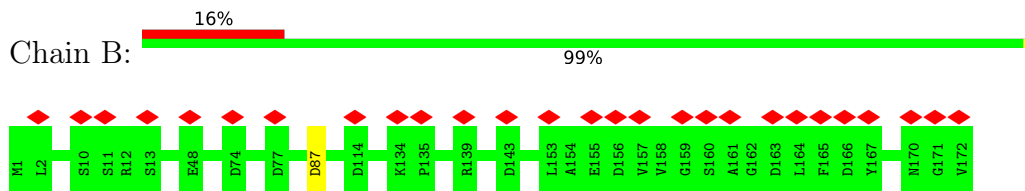




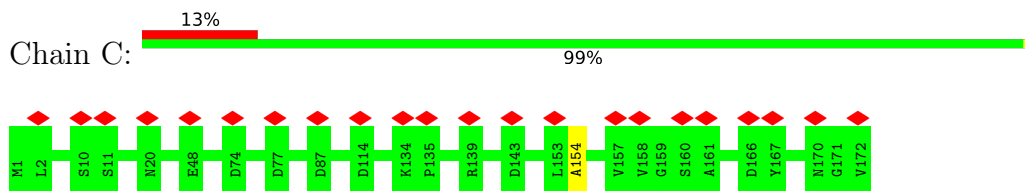
• Molecule 6: Baseplate component gp37



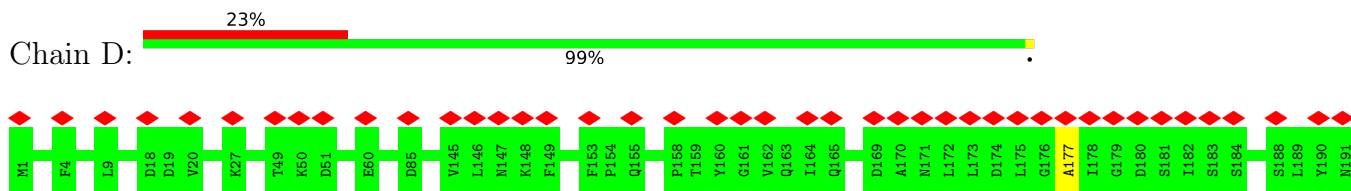
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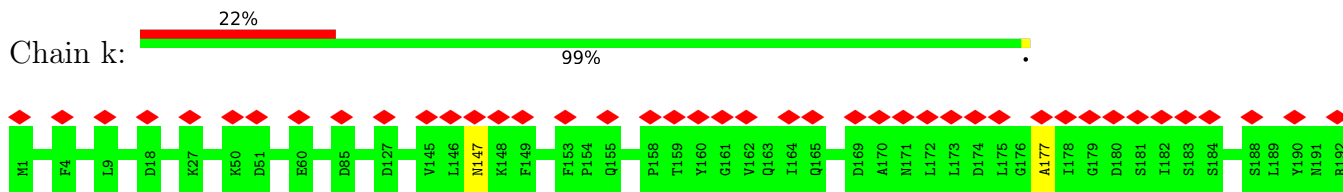


• Molecule 7: Baseplate component gp38



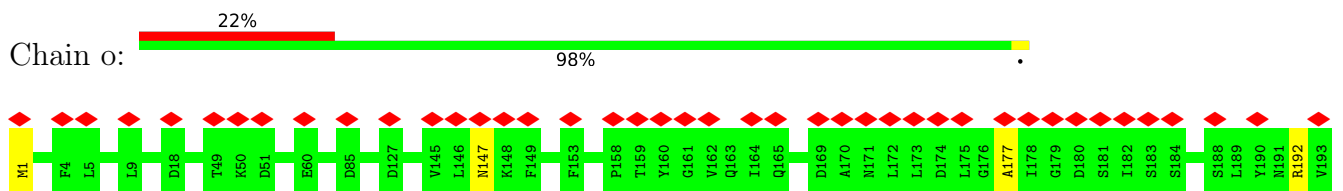
R192
V193

• Molecule 7: Baseplate component gp38

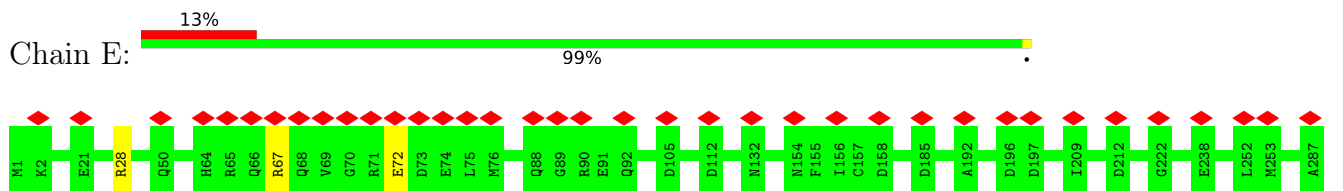


V193

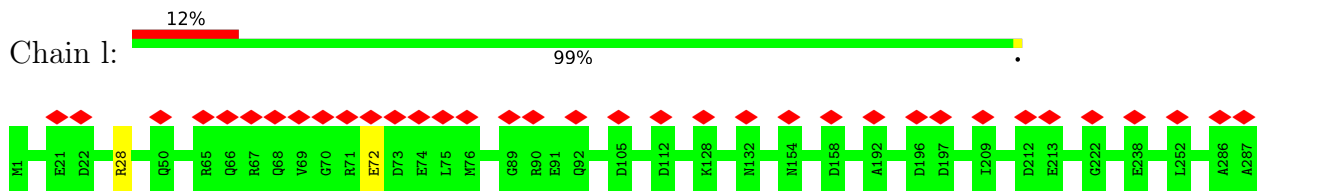
• Molecule 7: Baseplate component gp38



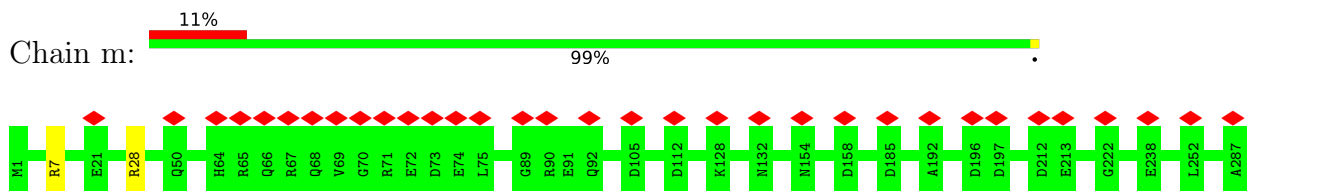
• Molecule 8: Baseplate hub gp41



• Molecule 8: Baseplate hub gp41

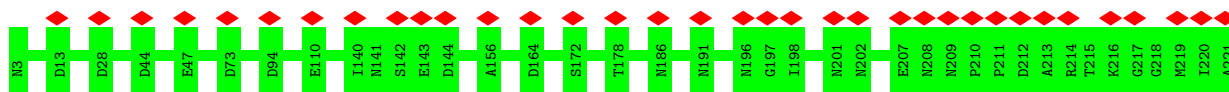


• Molecule 8: Baseplate hub gp41



• Molecule 9: Baseplate spike gp43

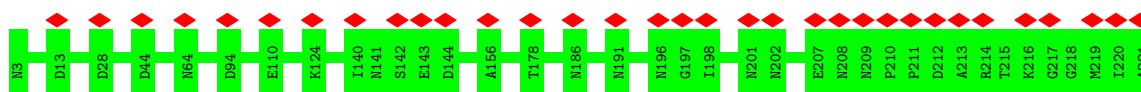




- Molecule 9: Baseplate spike gp43



- Molecule 9: Baseplate spike gp43



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	13.836	Depositor
Minimum map value	-6.766	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.36	Depositor
Map size (\AA)	448.0, 448.0, 448.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.12, 1.12, 1.12	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	G	0.32	0/839	0.54	0/1139
1	L	0.28	0/839	0.52	0/1139
1	Q	0.32	0/839	0.52	0/1139
1	V	0.30	0/839	0.52	0/1139
1	a	0.32	0/839	0.54	0/1139
1	f	0.30	0/839	0.52	0/1139
2	H	0.28	0/832	0.53	0/1128
2	M	0.29	0/832	0.53	0/1128
2	R	0.29	0/832	0.53	0/1128
2	W	0.28	0/832	0.56	0/1128
2	b	0.30	0/832	0.54	0/1128
2	g	0.27	0/832	0.53	0/1128
3	I	0.29	0/1155	0.55	0/1563
3	N	2.43	6/1155 (0.5%)	0.56	0/1563
3	S	0.31	0/1155	0.53	0/1563
3	X	3.35	6/1155 (0.5%)	0.56	2/1563 (0.1%)
3	c	0.30	0/1155	0.53	0/1563
3	h	0.29	0/1155	0.53	0/1563
4	J	0.28	0/3090	0.53	0/4225
4	O	0.29	0/3090	0.53	0/4225
4	T	0.28	0/3090	0.52	0/4225
4	Y	0.29	0/3090	0.54	0/4225
4	d	0.28	0/3090	0.53	0/4225
4	i	0.28	0/3090	0.53	0/4225
4	q	0.28	0/2986	0.53	0/4082
4	r	0.28	0/2986	0.53	0/4082
4	s	0.28	0/2986	0.54	0/4082
4	t	0.28	0/2985	0.54	0/4079
4	u	0.27	0/2985	0.53	0/4079
4	v	0.28	0/2985	0.53	0/4079
5	K	0.27	0/3922	0.54	0/5363
5	P	0.28	0/3922	0.54	0/5363
5	U	0.27	0/3922	0.53	0/5363
5	Z	0.37	2/3922 (0.1%)	0.61	5/5363 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	e	0.35	2/3922 (0.1%)	0.63	4/5363 (0.1%)
5	j	0.29	0/3922	0.55	1/5363 (0.0%)
6	A	0.54	2/1346 (0.1%)	0.74	5/1821 (0.3%)
6	B	0.29	0/1346	0.55	0/1821
6	C	0.28	0/1346	0.55	0/1821
7	D	0.27	0/1505	0.51	0/2049
7	k	0.28	0/1505	0.51	0/2049
7	o	1.23	1/1505 (0.1%)	0.70	3/2049 (0.1%)
8	E	0.30	0/2321	0.54	0/3145
8	l	0.29	0/2321	0.53	0/3145
8	m	0.30	0/2321	0.53	0/3145
9	F	0.28	0/1719	0.54	0/2339
9	n	0.28	0/1719	0.55	0/2339
9	p	0.28	0/1719	0.54	0/2339
All	All	0.56	19/97614 (0.0%)	0.55	20/133053 (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	1
1	L	0	1
1	Q	0	1
1	V	0	1
1	a	0	1
1	f	0	1
4	t	0	1
4	u	0	1
4	v	0	2
All	All	0	10

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	49	TYR	CD2-CE2	67.30	2.40	1.39
3	X	49	TYR	CD1-CE1	58.37	2.27	1.39
7	o	1	MET	CG-SD	46.17	3.01	1.81
3	N	146	TYR	CD2-CE2	43.93	2.05	1.39
3	N	146	TYR	CD1-CE1	41.58	2.01	1.39

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	221	PRO	N-CD-CG	-18.57	75.34	103.20
7	o	1	MET	CG-SD-CE	17.86	128.78	100.20
6	A	32	SER	C-N-CA	14.08	156.90	121.70
5	Z	413	PRO	N-CD-CG	-13.84	82.44	103.20
5	e	221	PRO	CA-CB-CG	-12.24	80.75	104.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	65	ARG	Peptide
1	L	65	ARG	Peptide
1	Q	65	ARG	Peptide
1	V	65	ARG	Peptide
1	a	65	ARG	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
1	L	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
1	Q	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
1	V	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
1	a	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
1	f	100/102 (98%)	94 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	106/108 (98%)	96 (91%)	7 (7%)	3 (3%)	5	34
2	M	106/108 (98%)	95 (90%)	8 (8%)	3 (3%)	5	34
2	R	106/108 (98%)	94 (89%)	10 (9%)	2 (2%)	8	42
2	W	106/108 (98%)	96 (91%)	8 (8%)	2 (2%)	8	42
2	b	106/108 (98%)	93 (88%)	11 (10%)	2 (2%)	8	42
2	g	106/108 (98%)	95 (90%)	9 (8%)	2 (2%)	8	42
3	I	150/152 (99%)	140 (93%)	8 (5%)	2 (1%)	12	50
3	N	150/152 (99%)	136 (91%)	14 (9%)	0	100	100
3	S	150/152 (99%)	136 (91%)	12 (8%)	2 (1%)	12	50
3	X	150/152 (99%)	140 (93%)	10 (7%)	0	100	100
3	c	150/152 (99%)	140 (93%)	9 (6%)	1 (1%)	22	61
3	h	150/152 (99%)	138 (92%)	10 (7%)	2 (1%)	12	50
4	J	415/417 (100%)	367 (88%)	48 (12%)	0	100	100
4	O	415/417 (100%)	371 (89%)	44 (11%)	0	100	100
4	T	415/417 (100%)	359 (86%)	56 (14%)	0	100	100
4	Y	415/417 (100%)	374 (90%)	41 (10%)	0	100	100
4	d	415/417 (100%)	352 (85%)	63 (15%)	0	100	100
4	i	415/417 (100%)	372 (90%)	43 (10%)	0	100	100
4	q	402/417 (96%)	346 (86%)	55 (14%)	1 (0%)	47	79
4	r	402/417 (96%)	340 (85%)	61 (15%)	1 (0%)	47	79
4	s	402/417 (96%)	349 (87%)	52 (13%)	1 (0%)	47	79
4	t	400/417 (96%)	354 (88%)	43 (11%)	3 (1%)	19	59
4	u	400/417 (96%)	352 (88%)	45 (11%)	3 (1%)	19	59
4	v	400/417 (96%)	356 (89%)	41 (10%)	3 (1%)	19	59
5	K	498/500 (100%)	450 (90%)	47 (9%)	1 (0%)	47	79
5	P	498/500 (100%)	445 (89%)	53 (11%)	0	100	100
5	U	498/500 (100%)	449 (90%)	49 (10%)	0	100	100
5	Z	498/500 (100%)	449 (90%)	49 (10%)	0	100	100
5	e	498/500 (100%)	452 (91%)	46 (9%)	0	100	100
5	j	498/500 (100%)	451 (91%)	47 (9%)	0	100	100
6	A	170/172 (99%)	147 (86%)	21 (12%)	2 (1%)	13	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	170/172 (99%)	147 (86%)	22 (13%)	1 (1%)	25	64
6	C	170/172 (99%)	152 (89%)	17 (10%)	1 (1%)	25	64
7	D	191/193 (99%)	161 (84%)	29 (15%)	1 (0%)	29	68
7	k	191/193 (99%)	162 (85%)	27 (14%)	2 (1%)	15	55
7	o	191/193 (99%)	162 (85%)	27 (14%)	2 (1%)	15	55
8	E	285/287 (99%)	268 (94%)	16 (6%)	1 (0%)	34	71
8	l	285/287 (99%)	267 (94%)	17 (6%)	1 (0%)	34	71
8	m	285/287 (99%)	269 (94%)	16 (6%)	0	100	100
9	F	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
9	n	217/219 (99%)	200 (92%)	17 (8%)	0	100	100
9	p	217/219 (99%)	199 (92%)	18 (8%)	0	100	100
All	All	12609/12789 (99%)	11288 (90%)	1276 (10%)	45 (0%)	38	71

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	89	PHE
3	c	89	PHE
3	h	89	PHE
6	A	87	ASP
6	A	153	LEU

5.3.2 Protein sidechains [i](#)

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	G	84/84 (100%)	83 (99%)	1 (1%)	71	87
1	L	84/84 (100%)	84 (100%)	0	100	100
1	Q	84/84 (100%)	84 (100%)	0	100	100
1	V	84/84 (100%)	83 (99%)	1 (1%)	71	87
1	a	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	84/84 (100%)	84 (100%)	0	100	100
2	H	92/92 (100%)	92 (100%)	0	100	100
2	M	92/92 (100%)	92 (100%)	0	100	100
2	R	92/92 (100%)	92 (100%)	0	100	100
2	W	92/92 (100%)	92 (100%)	0	100	100
2	b	92/92 (100%)	92 (100%)	0	100	100
2	g	92/92 (100%)	92 (100%)	0	100	100
3	I	124/124 (100%)	124 (100%)	0	100	100
3	N	124/124 (100%)	124 (100%)	0	100	100
3	S	124/124 (100%)	124 (100%)	0	100	100
3	X	124/124 (100%)	124 (100%)	0	100	100
3	c	124/124 (100%)	123 (99%)	1 (1%)	81	91
3	h	124/124 (100%)	124 (100%)	0	100	100
4	J	320/320 (100%)	318 (99%)	2 (1%)	86	94
4	O	320/320 (100%)	319 (100%)	1 (0%)	92	97
4	T	320/320 (100%)	320 (100%)	0	100	100
4	Y	320/320 (100%)	316 (99%)	4 (1%)	69	86
4	d	320/320 (100%)	318 (99%)	2 (1%)	86	94
4	i	320/320 (100%)	319 (100%)	1 (0%)	92	97
4	q	309/320 (97%)	308 (100%)	1 (0%)	92	97
4	r	309/320 (97%)	308 (100%)	1 (0%)	92	97
4	s	309/320 (97%)	309 (100%)	0	100	100
4	t	309/320 (97%)	308 (100%)	1 (0%)	92	97
4	u	309/320 (97%)	309 (100%)	0	100	100
4	v	309/320 (97%)	309 (100%)	0	100	100
5	K	404/404 (100%)	404 (100%)	0	100	100
5	P	404/404 (100%)	404 (100%)	0	100	100
5	U	404/404 (100%)	404 (100%)	0	100	100
5	Z	404/404 (100%)	403 (100%)	1 (0%)	93	98
5	e	404/404 (100%)	404 (100%)	0	100	100
5	j	404/404 (100%)	403 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	153/153 (100%)	153 (100%)	0	100	100
6	B	153/153 (100%)	153 (100%)	0	100	100
6	C	153/153 (100%)	153 (100%)	0	100	100
7	D	173/173 (100%)	173 (100%)	0	100	100
7	k	173/173 (100%)	173 (100%)	0	100	100
7	o	173/173 (100%)	172 (99%)	1 (1%)	86	94
8	E	252/252 (100%)	250 (99%)	2 (1%)	81	91
8	l	252/252 (100%)	251 (100%)	1 (0%)	91	97
8	m	252/252 (100%)	250 (99%)	2 (1%)	81	91
9	F	184/184 (100%)	184 (100%)	0	100	100
9	n	184/184 (100%)	184 (100%)	0	100	100
9	p	184/184 (100%)	184 (100%)	0	100	100
All	All	10284/10350 (99%)	10260 (100%)	24 (0%)	93	98

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	j	246	LYS
8	l	28	ARG
8	E	67	ARG
8	m	7	ARG
4	Y	203	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
9	n	53	GLN
4	t	150	ASN
9	n	92	GLN
9	p	203	HIS
4	u	150	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	v	1
4	u	1
4	t	1
6	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	68:THR	C	69:ILE	N	6.21
1	u	68:THR	C	69:ILE	N	6.20
1	t	68:THR	C	69:ILE	N	6.19
1	A	32:SER	C	33:ARG	N	1.63

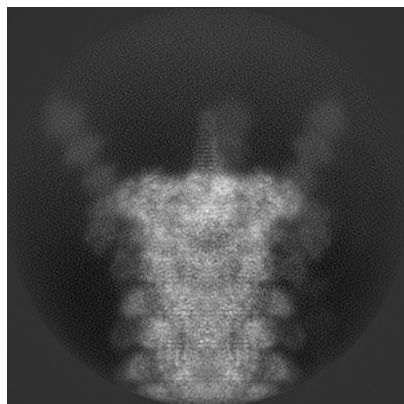
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28405. These allow visual inspection of the internal detail of the map and identification of artifacts.

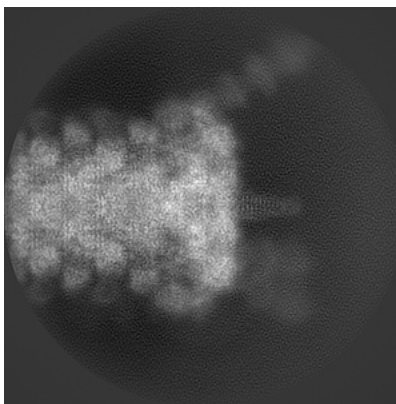
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

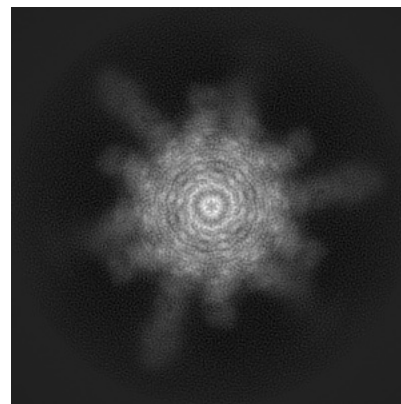
6.1.1 Primary map



X

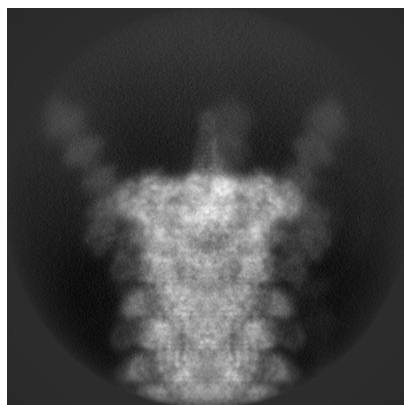


Y

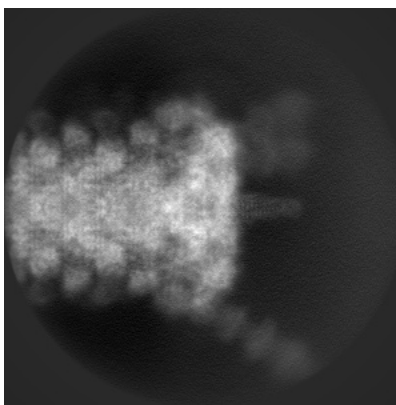


Z

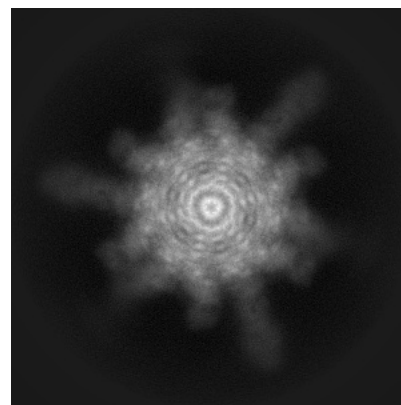
6.1.2 Raw map



X



Y

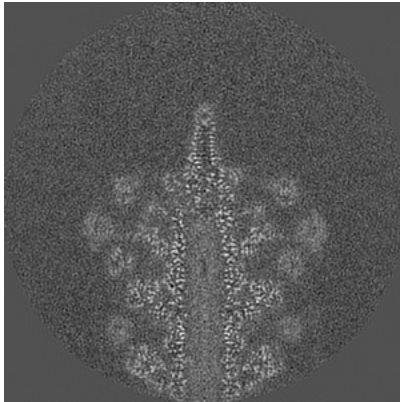


Z

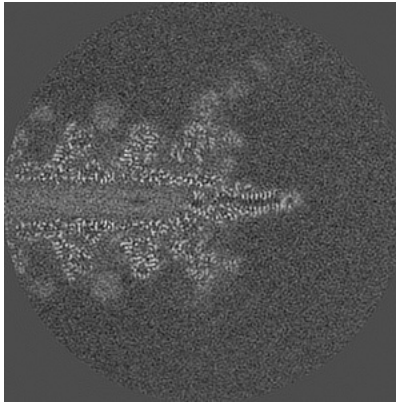
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

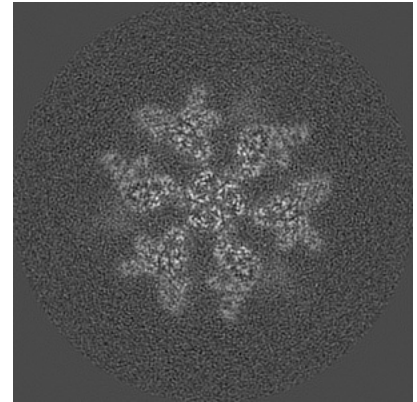
6.2.1 Primary map



X Index: 200

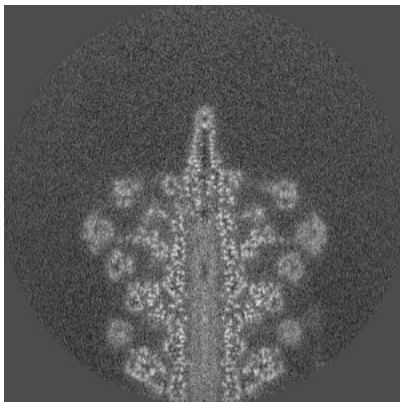


Y Index: 200

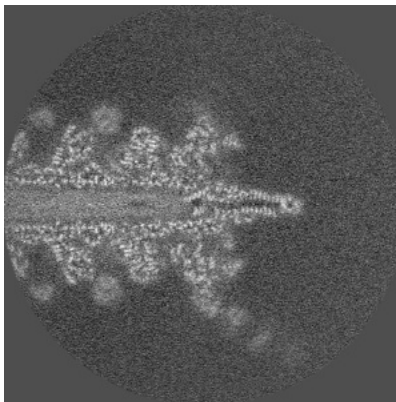


Z Index: 200

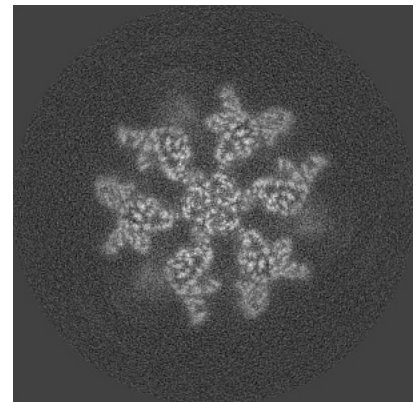
6.2.2 Raw map



X Index: 200



Y Index: 200

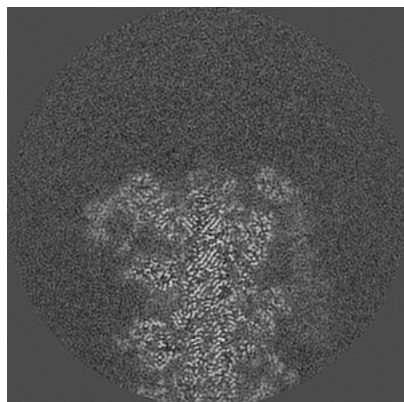


Z Index: 200

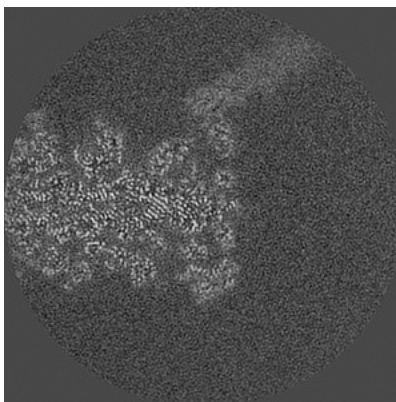
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

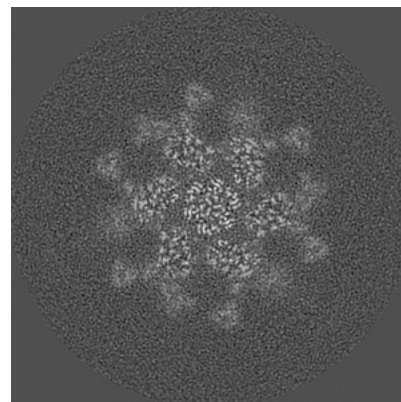
6.3.1 Primary map



X Index: 220

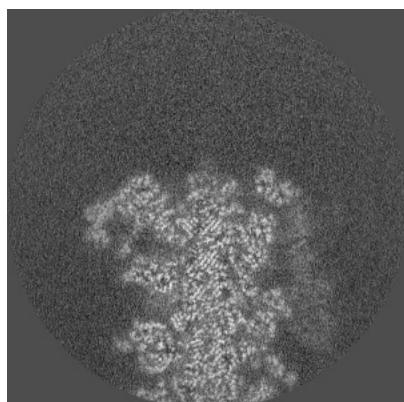


Y Index: 219

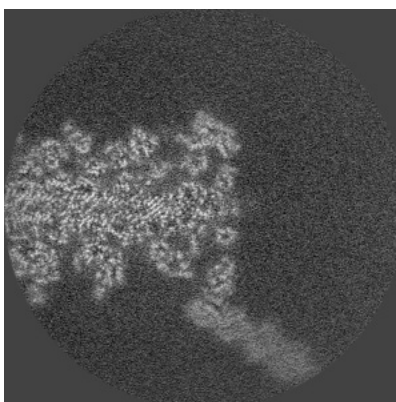


Z Index: 191

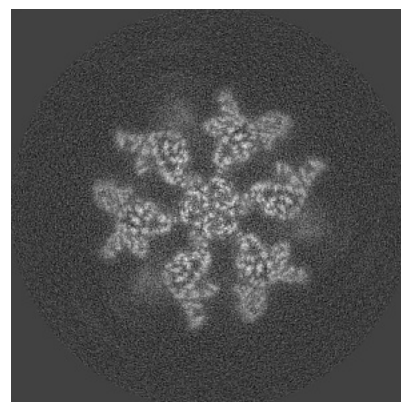
6.3.2 Raw map



X Index: 180



Y Index: 220

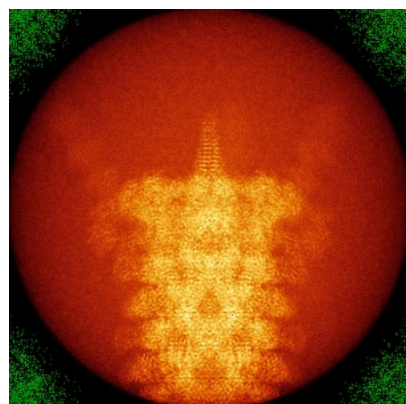


Z Index: 200

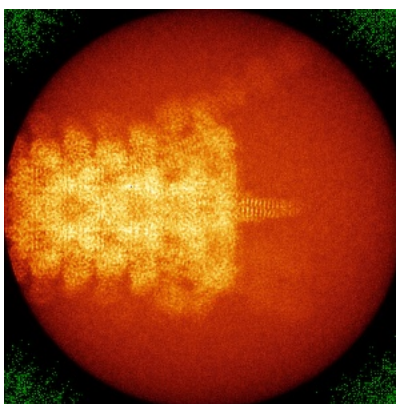
The images above show the largest variance slices of the map in three orthogonal directions.

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

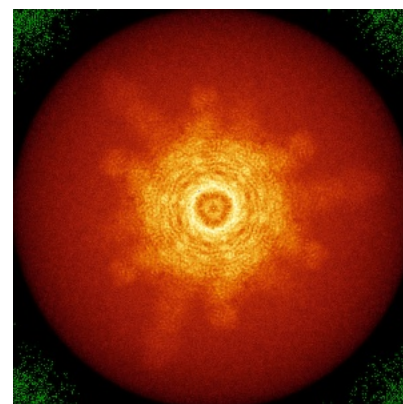
6.4.1 Primary map



X

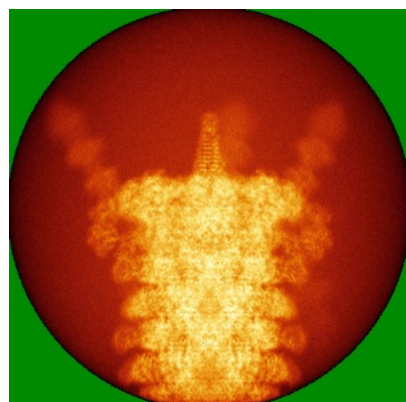


Y

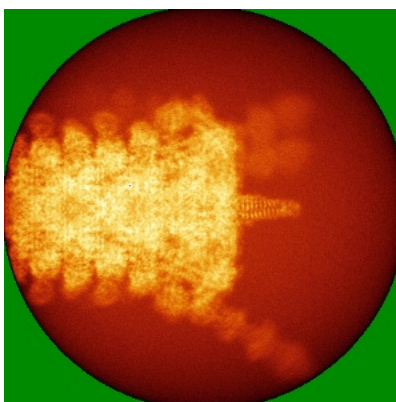


Z

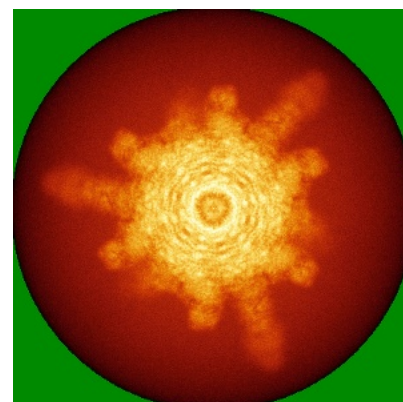
6.4.2 Raw map



X



Y

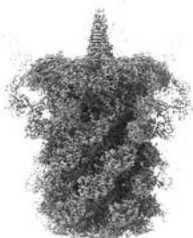


Z

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

6.5 Orthogonal surface views [i](#)

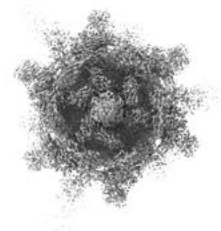
6.5.1 Primary map



X



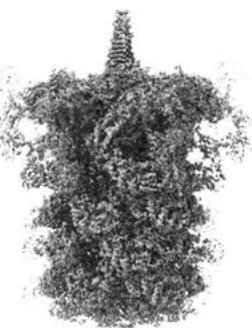
Y



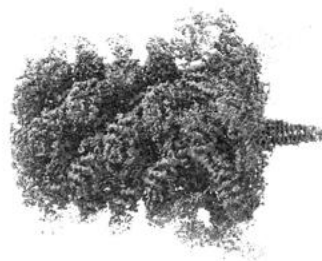
Z

The images above show the 3D surface view of the map at the recommended contour level 4.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

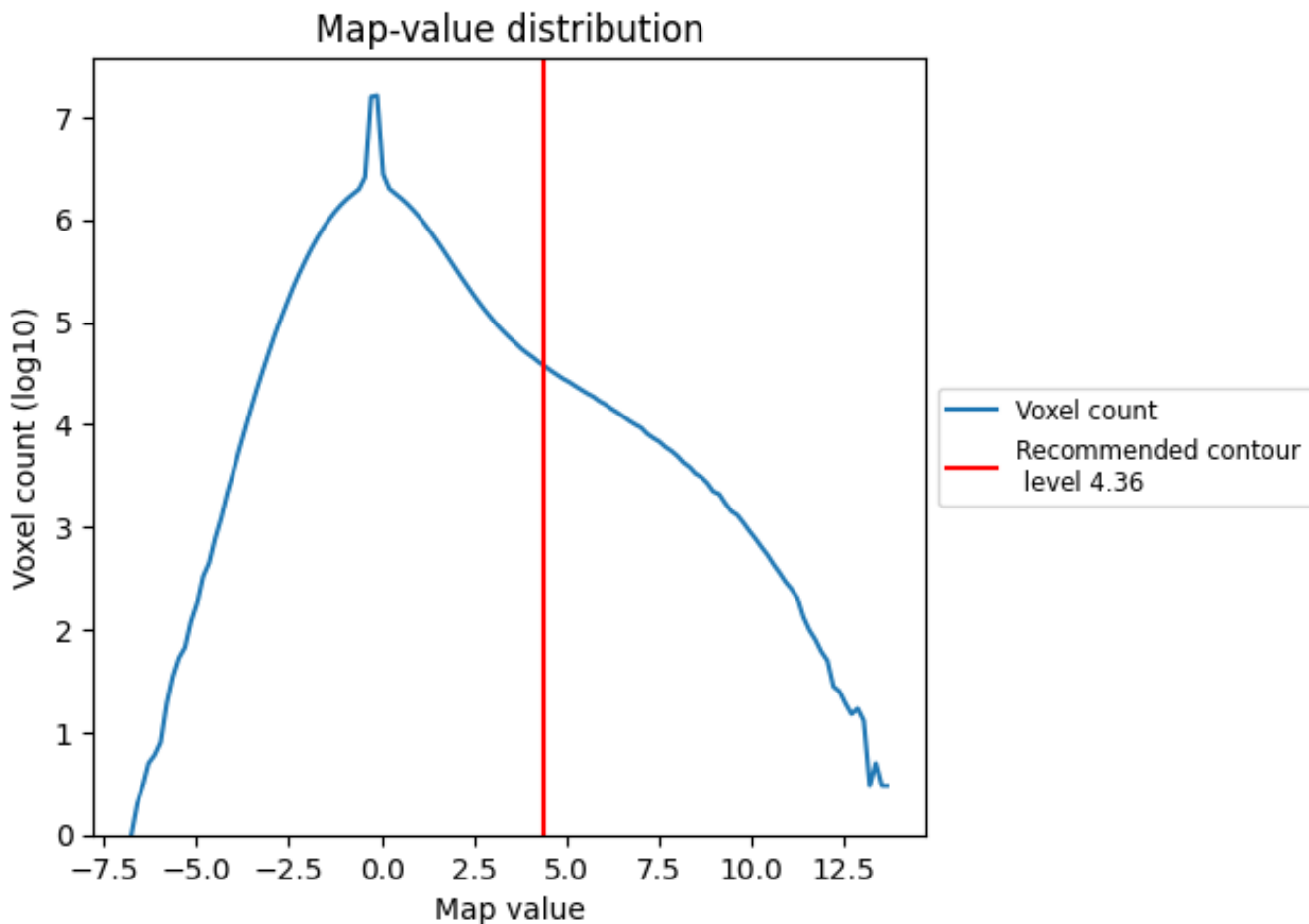
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

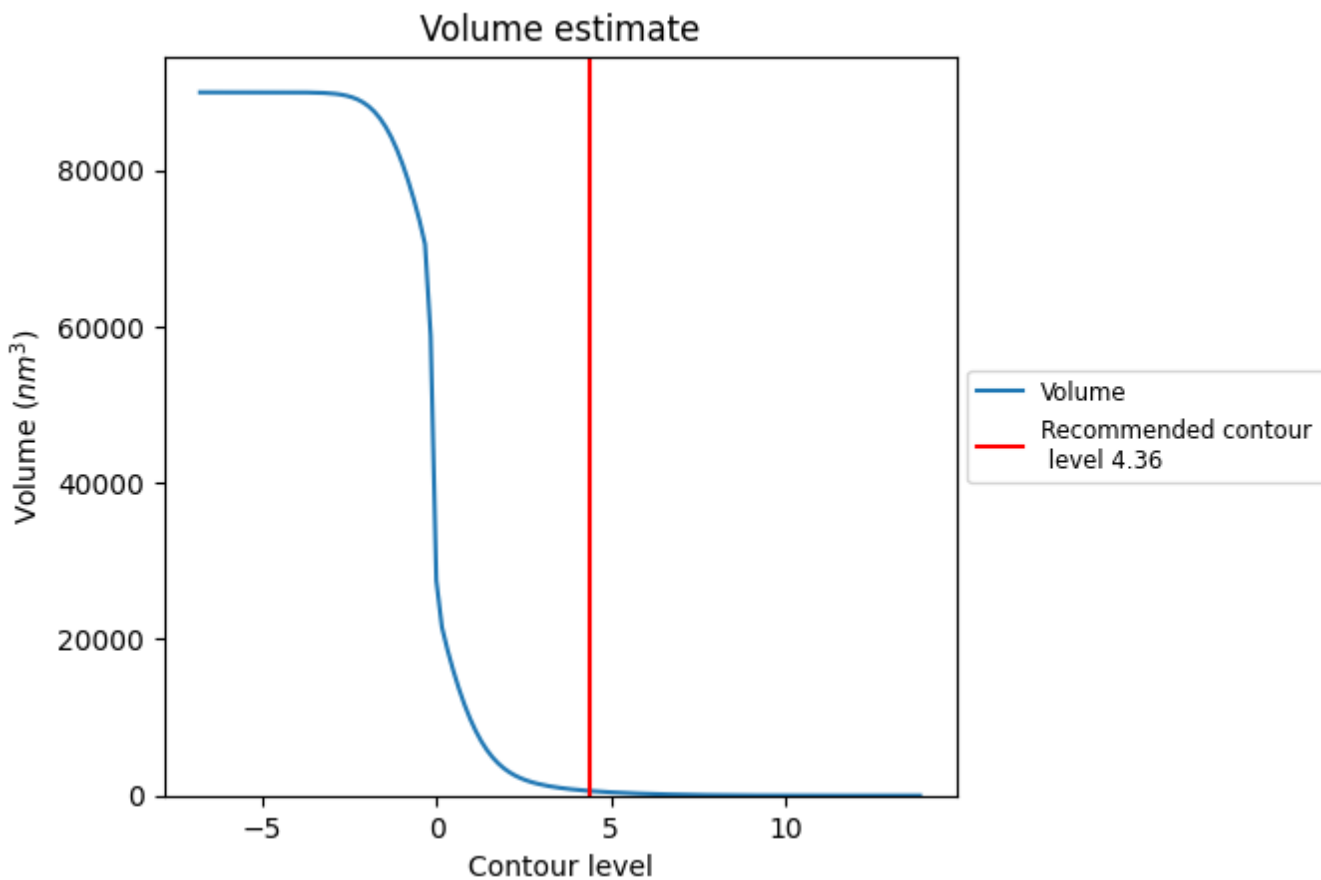
This section contains the results of statistical analysis of the map.

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.

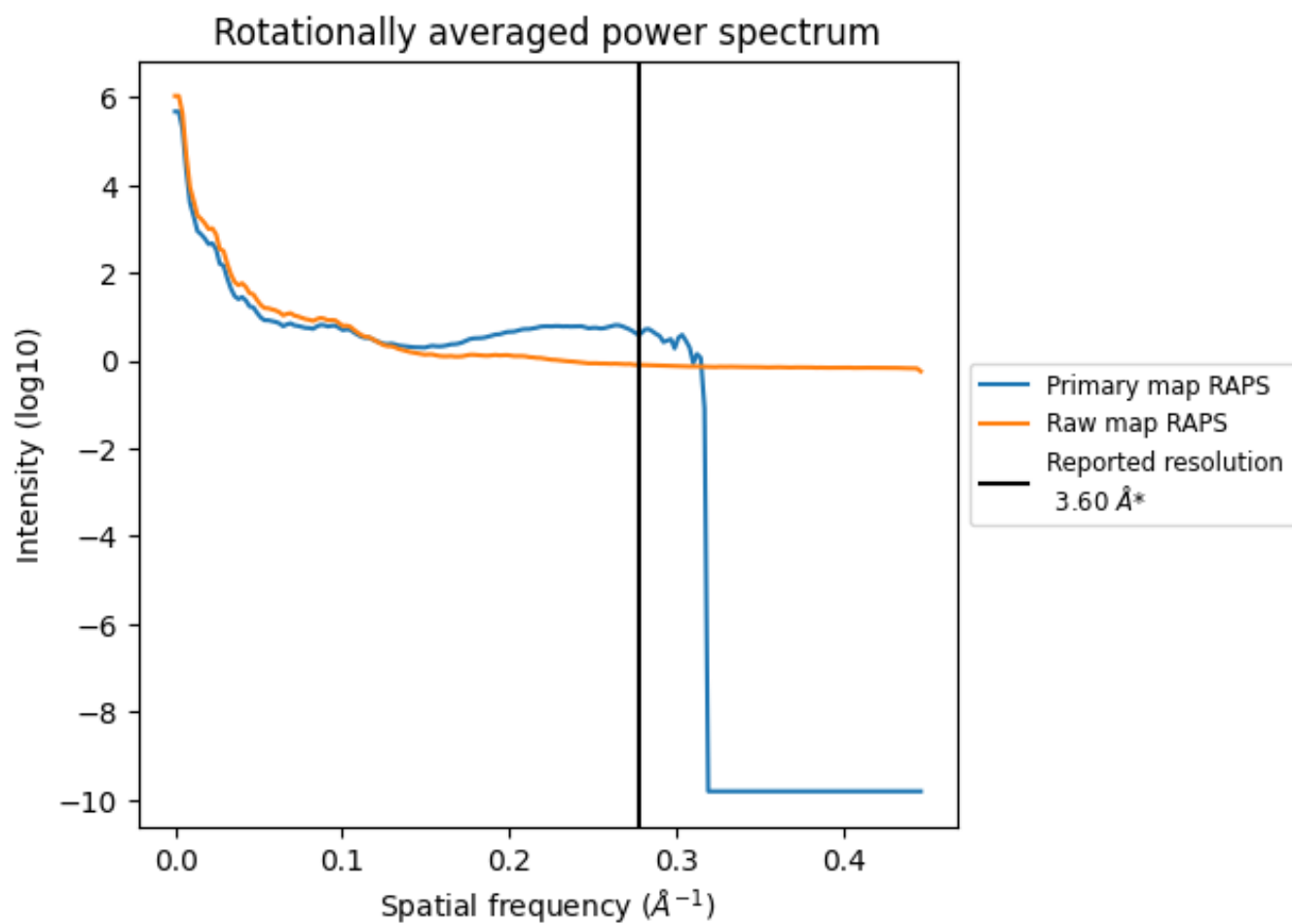
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 602 nm^3 ; this corresponds to an approximate mass of 544 kDa.

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

7.3 Rotationally averaged power spectrum i

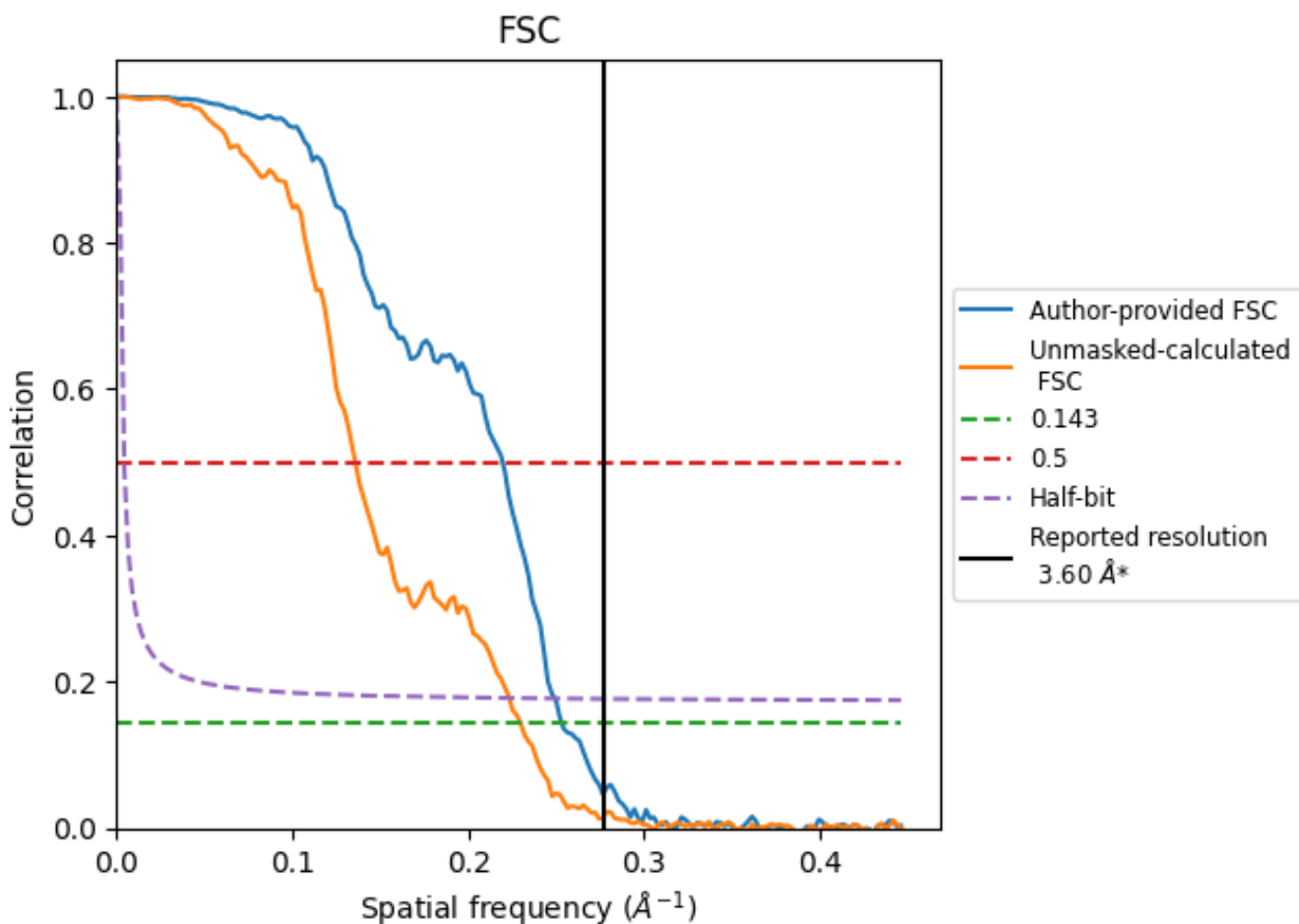


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

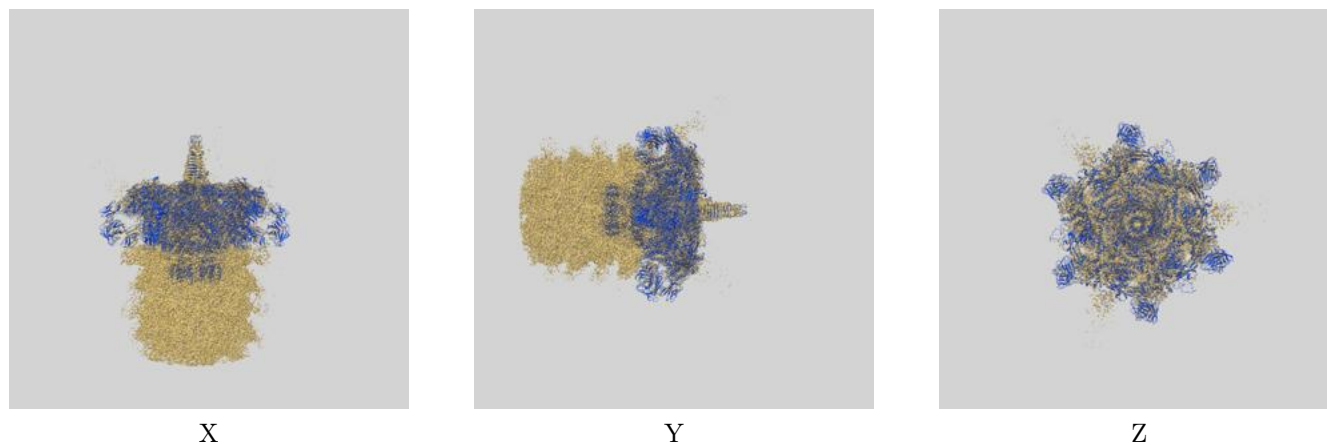
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.95	4.55	4.01
Unmasked-calculated*	4.35	7.36	4.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

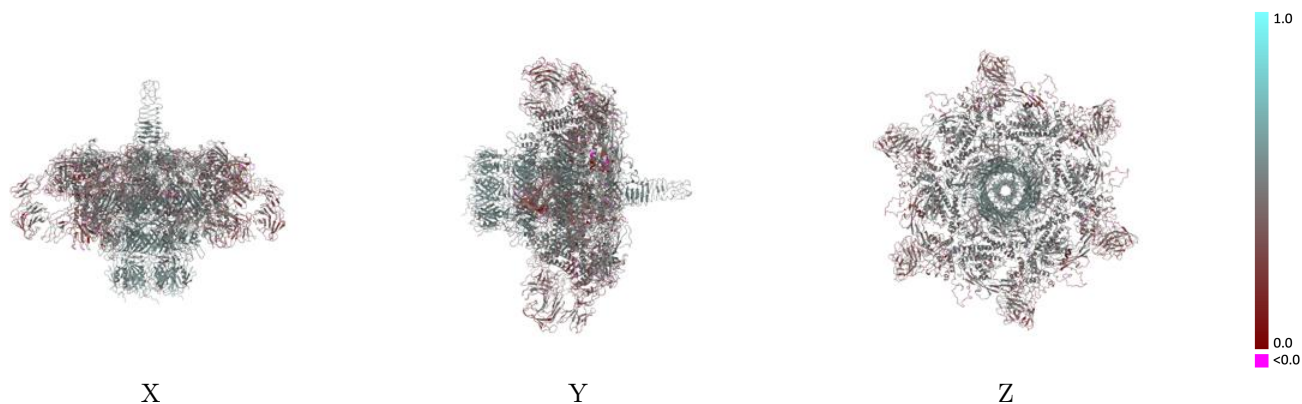
This section contains information regarding the fit between EMDB map EMD-28405 and PDB model 8EON. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



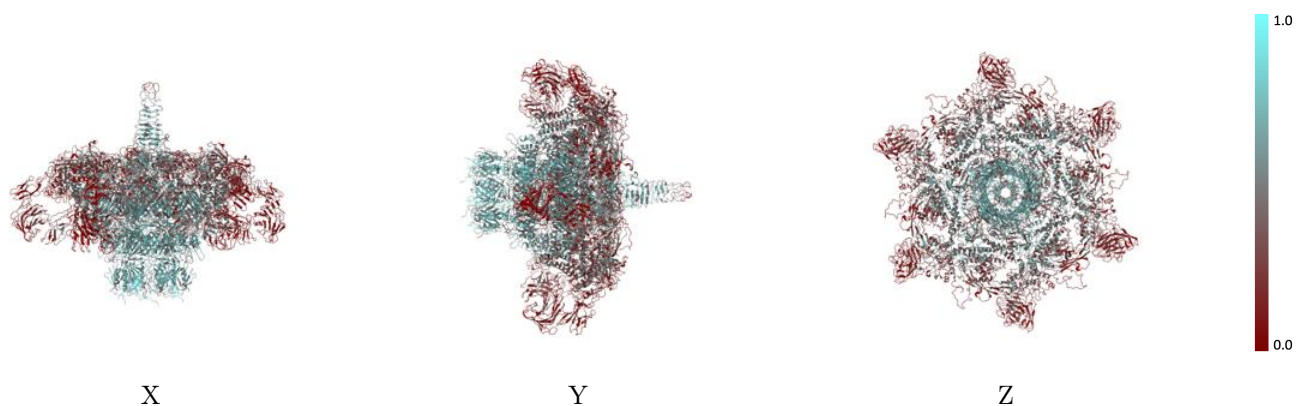
The images above show the 3D surface view of the map at the recommended contour level 4.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



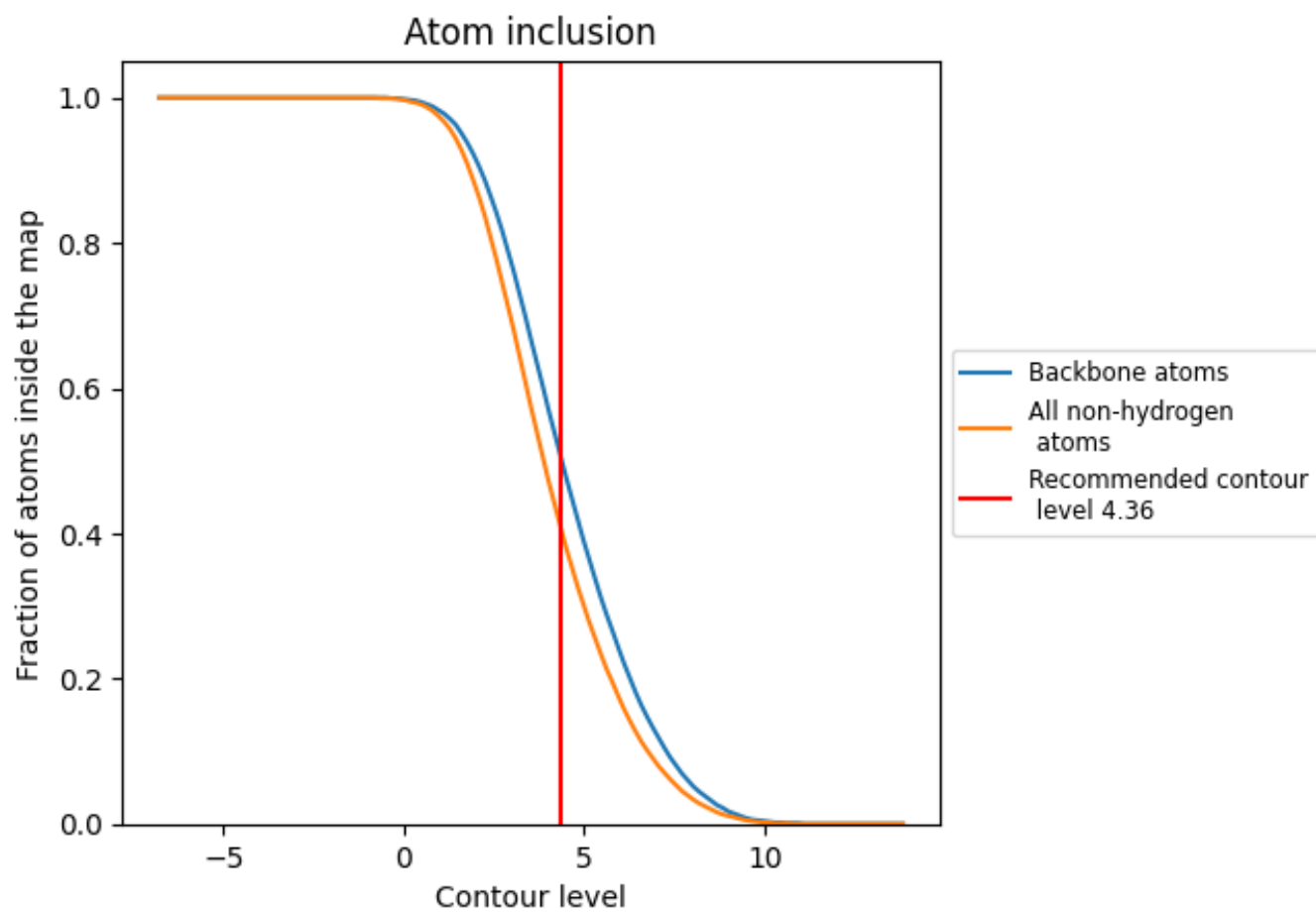
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.36).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 41% 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 (4.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4070	 0.4390
A	 0.6420	 0.5300
B	 0.6450	 0.5330
C	 0.6520	 0.5380
D	 0.5710	 0.5060
E	 0.6430	 0.5340
F	 0.6110	 0.5280
G	 0.6350	 0.5140
H	 0.5490	 0.4990
I	 0.6510	 0.5300
J	 0.3290	 0.4090
K	 0.1980	 0.3660
L	 0.5270	 0.4890
M	 0.5850	 0.4980
N	 0.6190	 0.5140
O	 0.3030	 0.3720
P	 0.1850	 0.3490
Q	 0.6310	 0.5080
R	 0.5720	 0.4950
S	 0.6540	 0.5340
T	 0.3320	 0.4070
U	 0.1950	 0.3710
V	 0.5270	 0.4750
W	 0.5430	 0.4950
X	 0.6230	 0.5240
Y	 0.2880	 0.3660
Z	 0.1740	 0.3410
a	 0.6350	 0.5080
b	 0.5800	 0.4940
c	 0.6200	 0.5270
d	 0.3290	 0.4060
e	 0.1950	 0.3610
f	 0.5340	 0.4850
g	 0.5430	 0.4960
h	 0.6520	 0.5310



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Chain	Atom inclusion	Q-score
i	 0.2980	 0.3770
j	 0.1730	 0.3400
k	 0.5680	 0.5110
l	 0.6420	 0.5360
m	 0.6500	 0.5400
n	 0.6110	 0.5280
o	 0.5660	 0.5080
p	 0.6130	 0.5290
q	 0.3740	 0.4430
r	 0.3680	 0.4450
s	 0.3730	 0.4460
t	 0.3490	 0.4200
u	 0.3510	 0.4220
v	 0.3500	 0.4260