



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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

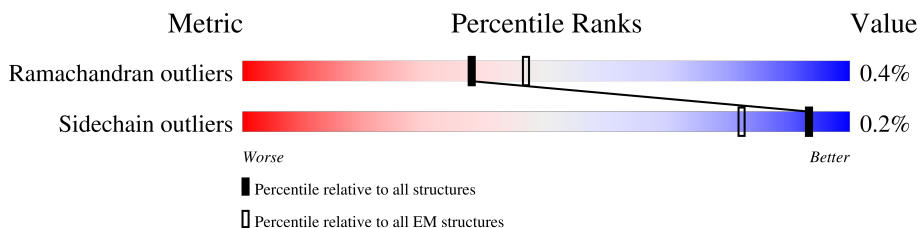
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

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

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

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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	<div>82%</div> <div>100%</div>
5	j	500	<div>85%</div> <div>100%</div>
6	A	172	<div>14%</div> <div>98%</div>
6	B	172	<div>16%</div> <div>99%</div>
6	C	172	<div>13%</div> <div>99%</div>
7	D	193	<div>23%</div> <div>99%</div>
7	k	193	<div>22%</div> <div>99%</div>
7	o	193	<div>22%</div> <div>98%</div>
8	E	287	<div>13%</div> <div>99%</div>
8	l	287	<div>12%</div> <div>99%</div>
8	m	287	<div>11%</div> <div>99%</div>
9	F	219	<div>16%</div> <div>100%</div>
9	n	219	<div>16%</div> <div>100%</div>
9	p	219	<div>15%</div> <div>100%</div>

2 Entry composition

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
1	G	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	L	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	Q	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	V	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	a	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	f	102	Total	C	N	O	S	0	0
			816	525	136	150	5		

- Molecule 2 is a protein called Baseplate component gp34.

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

- Molecule 3 is a protein called Baseplate component gp36.

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

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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		

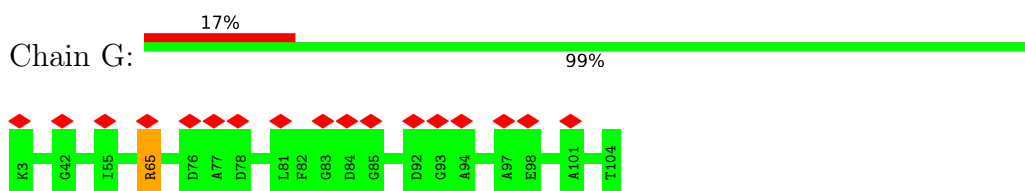
- Molecule 9 is a protein called Baseplate spike gp43.

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

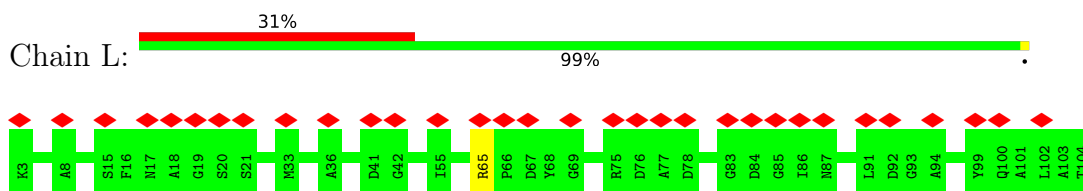
3 Residue-property plots [i](#)

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.

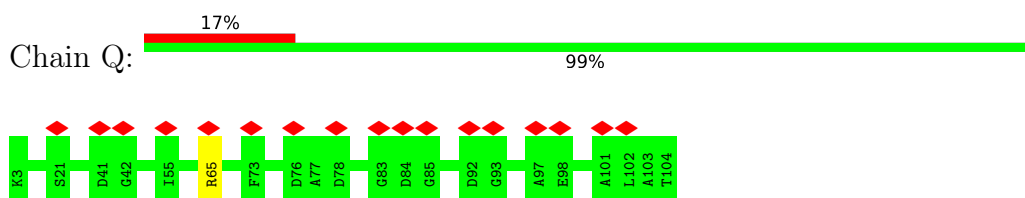
- Molecule 1: Baseplate component gp33



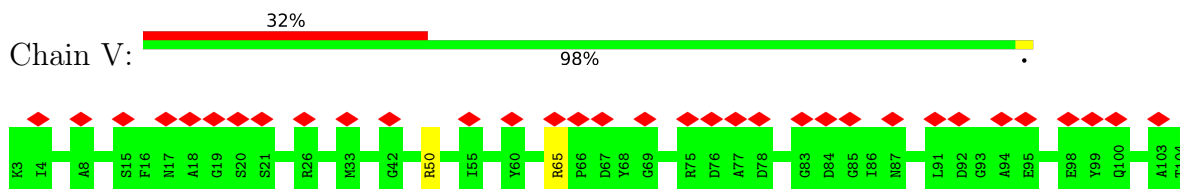
- Molecule 1: Baseplate component gp33



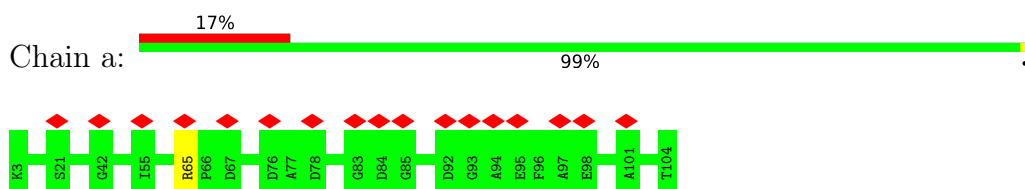
- Molecule 1: Baseplate component gp33



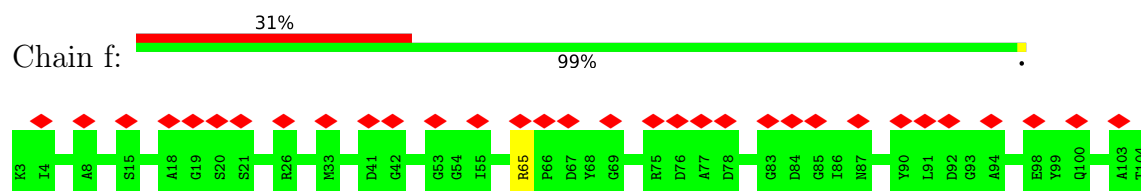
- Molecule 1: Baseplate component gp33



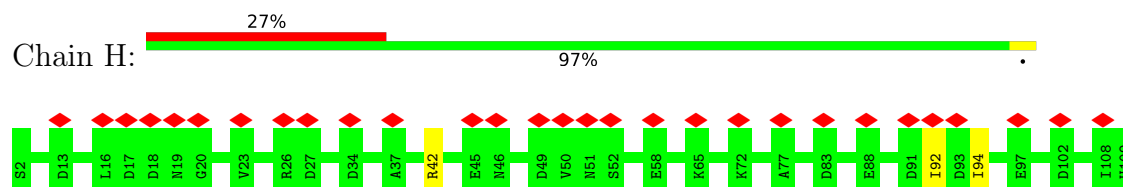
- Molecule 1: Baseplate component gp33



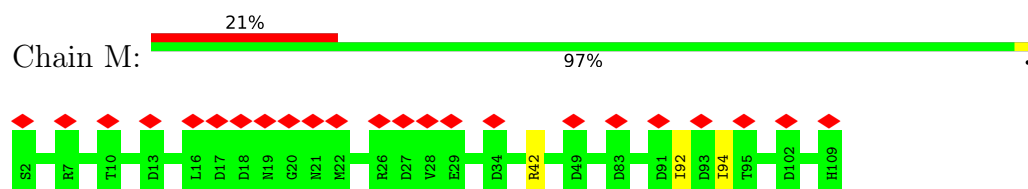
- Molecule 1: Baseplate component gp33



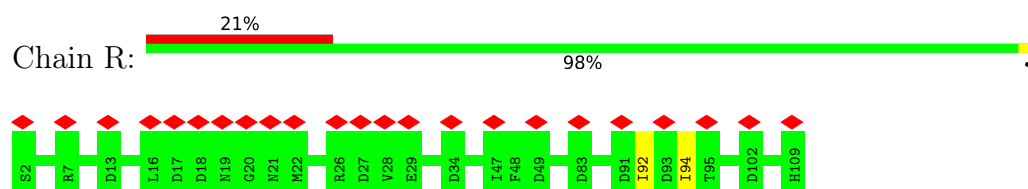
- Molecule 2: Baseplate component gp34



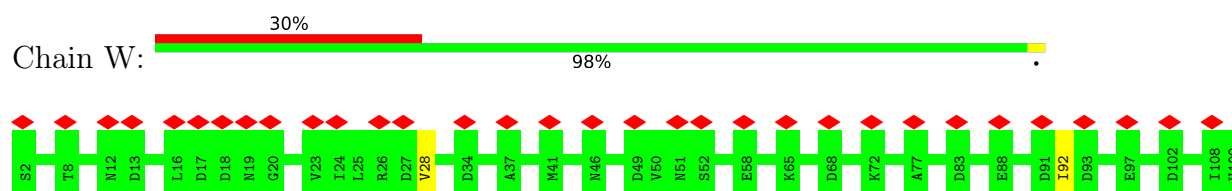
- Molecule 2: Baseplate component gp34



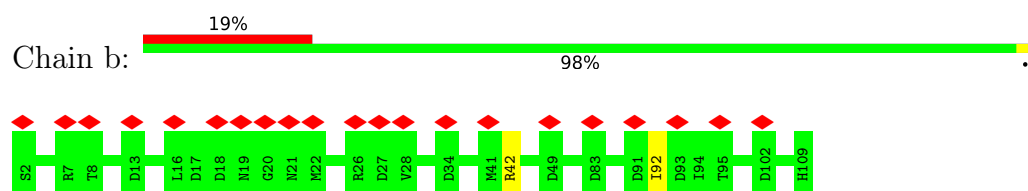
- Molecule 2: Baseplate component gp34



- Molecule 2: Baseplate component gp34

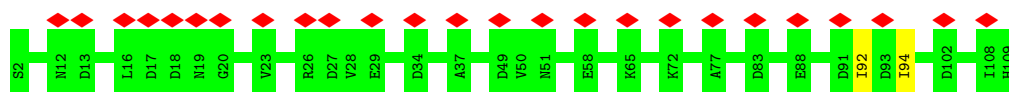


- Molecule 2: Baseplate component gp34

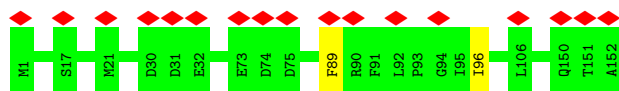


- Molecule 2: Baseplate component gp34

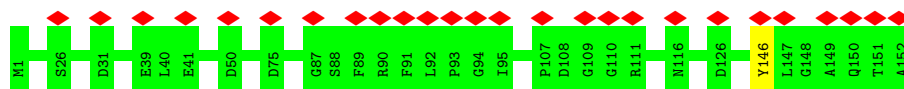




- Molecule 3: Baseplate component gp36



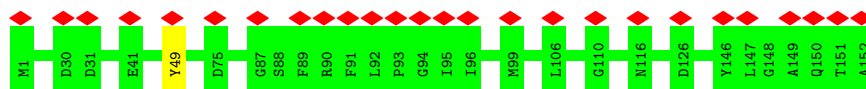
- Molecule 3: Baseplate component gp36



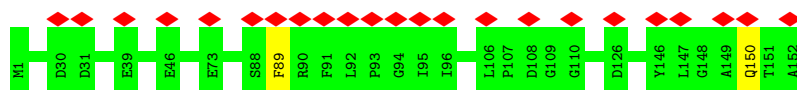
- Molecule 3: Baseplate component gp36



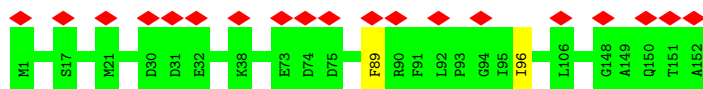
- Molecule 3: Baseplate component gp36



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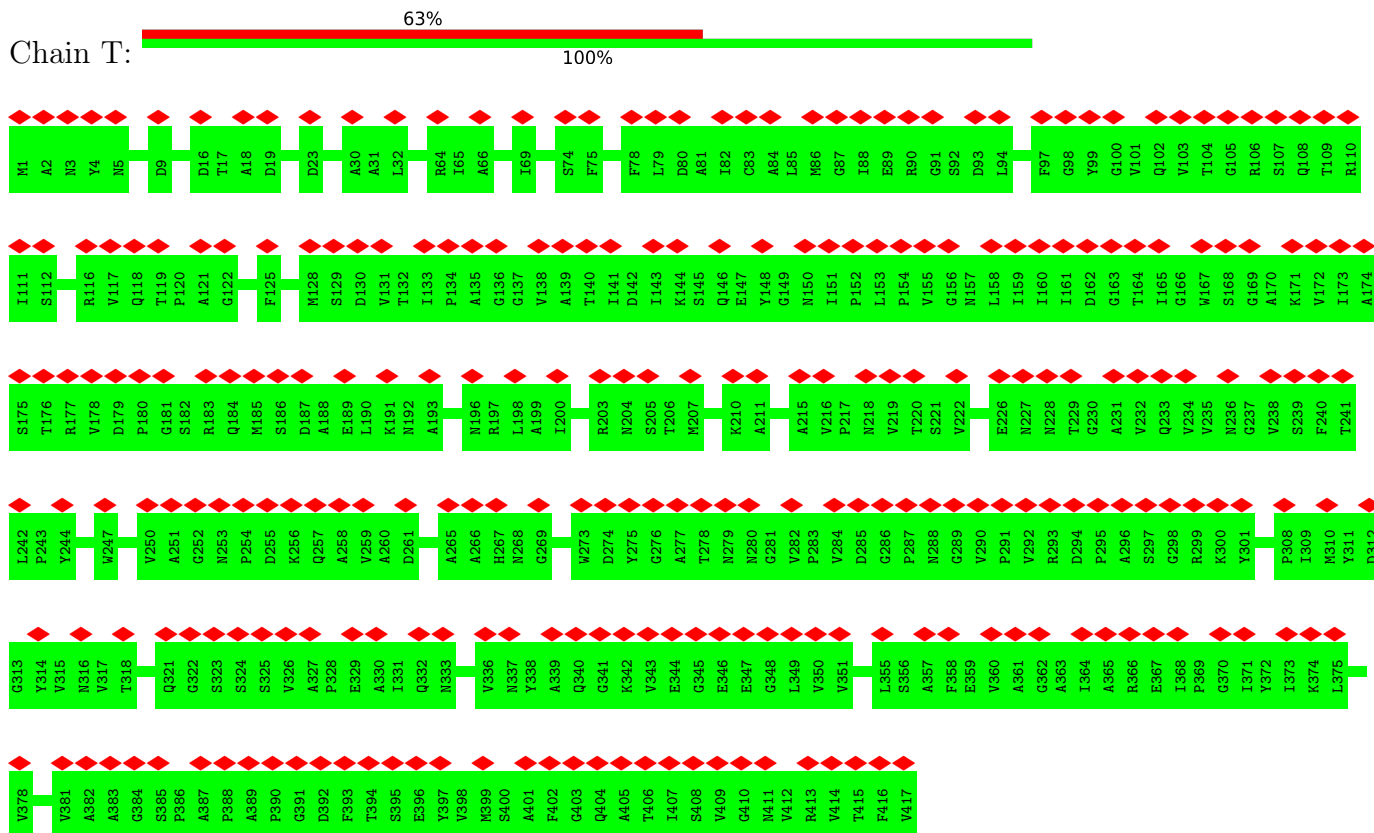


- Molecule 4: Triplex gp44-b

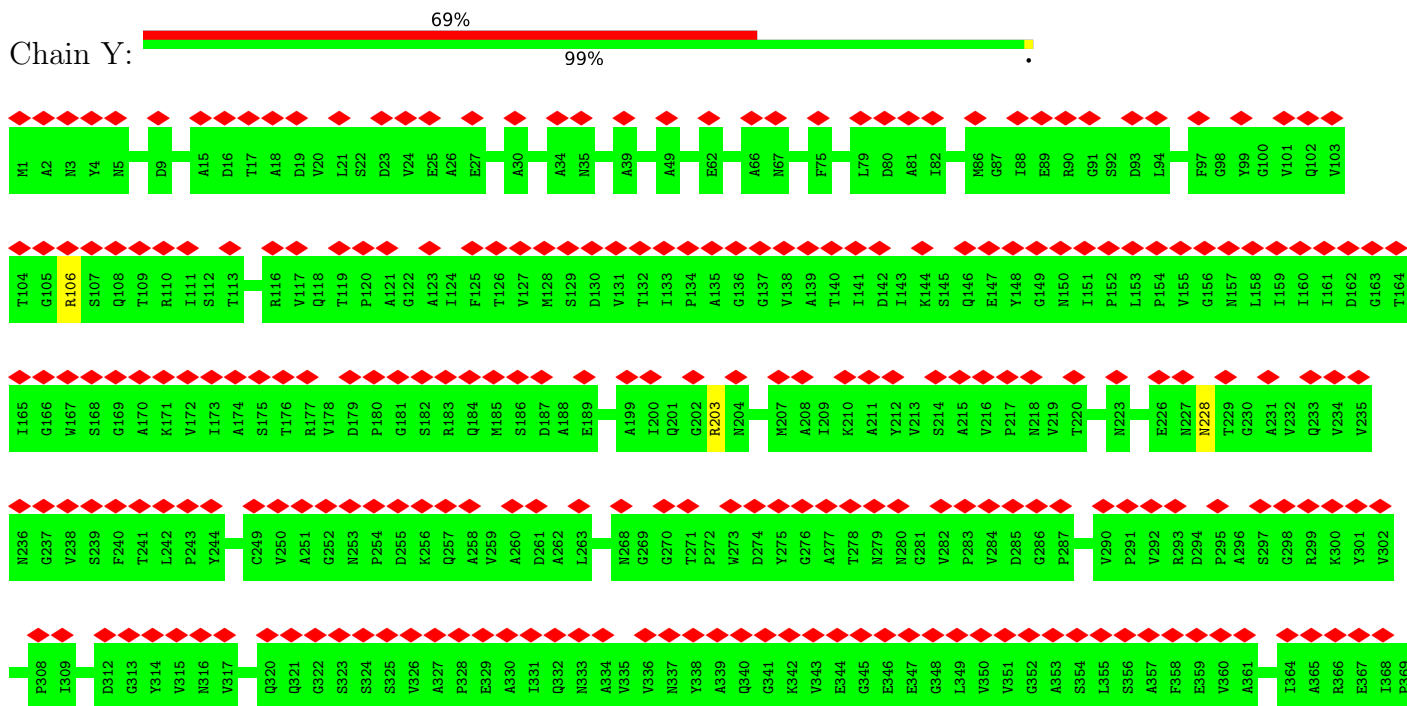
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P388	S325	P254	D179		A2
A389	V326	D255	P180	V117	N3
P390	A327	K256	G181	Q118	Y4
G391	F328	Q257	S182	T119	N5
D392	E329	A258	R183	P120	
F393	A330		Q184	A121	D9
T394	I331	D261	M185	G122	
S395	Q332				D16
E396	N333	A265	S186	V127	T17
F397	A334	A266	D187	M128	A18
V398	V335	H267	E188	S129	D19
K399	V336	N268	L190	D130	
S400	N337	G269	K191	V131	D23
A401	F338		M192	T132	
F402	A339	W273	A193	I133	A30
G403	Q340	D274		P134	A31
Q404	G341	Y275	L198	A135	L32
A405	K342	G276		G136	G45
T406	V343	A277	G202	G137	
I407	E344	T278	R203	V138	H64
S408	G345	N279	H204	A139	I65
V409	E346	N280	S205	T140	A66
G410	E347	G281	T206	I141	
N411	G348	V282	H207	D142	I69
V412	L349	P283		I143	F75
R413	V350	D284	K210	K144	
V414	V351	D285	A211	S145	L79
T415		G286	V212	Q146	D80
F416	L355	S356	V213	E147	A81
V417	A357	N287	S214	Y148	I82
	A357	G289	A215	G149	C83
	F358	V290	V216	P217	
	E359	P291	N218	I151	H86
	V360	V292	V219	P152	Q87
	A361	R293	T220	L153	I88
	G362	D294		P154	E89
	A363	P295	E226	V155	R90
	I364	A296	H227	G156	G91
	A365	S297	N228	M157	S92
	R366	G298	T229	L158	D93
	E367	R299		I159	I94
	I368	K300	Q233	I160	
	P369	Y301		I161	F97
	G370		H236	D162	G98
	I371	P308	G237	G163	Y99
	Y372	I309	V238	T164	G100
	I373	M310	S239	I165	V101
	K374	V311	F240	G166	Q102
	L375	D312	T241	W167	T103
	G376	G313	L242	S168	V104
	Q377	V314	P243	G169	G105
	V378	V315	Y244	A170	R106
		N316		K171	S107
	V381	V317	W247	V172	Q108
	A382	T318		I173	T109
	A383		V250	A174	R110
	G384	Q321	A251	S175	I111
	S385	G322	G252	T176	
	P386	S323		R177	

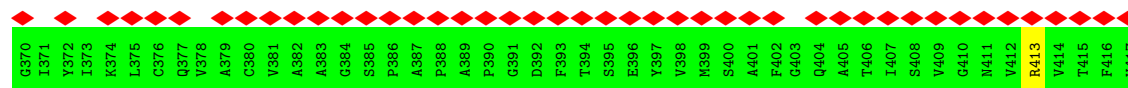
C380	C381	A382	A383	A384	S385	S386	A387	A389	P390	G391	D392	F393	T394	S395	E396	Y397	M399	S400	A401	F402	G403	Q404	A405	T406	I407	S408	V409	G410	N411	V412	R413	V414	T415	F416	V417																					
T318	V319	Q320	Q321	G322	S323	S324	S325	V326	A327	F328	E329	A330	I331	Q332	N333	V336	N337	Y338	A339	Q340	G341	K342	V343	E344	G345	E346	E347	G348	L349	V350	V351	Q352	A353	S354	L355	A357	F358	E359	V360	A361	I364	A365	R366	E367	I368	P369	G370	I371	Y372	I373	K374	L375	C376	Q377	V378	A379
C249	V250	A251	G252	N253	P254	D255	K256	Q257	A260	D261	A262	L263	A266	G269	G270	T271	P272	Q273	D274	V275	G276	A277	Z278	N279	N280	P283	V284	D285	G286	P287	V290	P291	V292	R293	D294	P295	G298	R299	K300	Y301	V302	P308	I309	M310	Y311	D312	G313	Y314	V315	N316	V317					
I173	A174	S175	T176	V177	V178	D179	P180	G181	S182	R183	Q184	M185	S186	D187	A188	E189	L190	K191	N192	A199	I200	Q201	G202	R203	N204	R207	A208	A211	S214	A215	V216	P217	N218	V219	T220	E226	N227	N228	T229	G230	A231	V232	Q233	V234	V235	N236	G237	V238	S239	F240	T241	L242	P243	Y244		
T109	R110	I111	S112	T113	R116	V117	Q118	T119	P120	A121	F125	T126	V127	M128	D130	V131	T132	I133	P134	A135	G136	G137	V138	A139	T140	I141	D142	S145	Q146	E147	V148	G149	N150	I151	P152	L153	P154	V155	G156	N157	L158	I159	I160	I161	D162	G163	T164	I165	G166	W167	S168	G169	A170	K171	V172	
M1	A2	N3	Y4	N5	D9	A15	D16	T17	D19	V20	L21	S22	D23	V24	E25	A26	E27	A30	A34	A39	E62	N67	F75	L79	I82	M86	G87	I88	E89	R90	G91	S92	D93	I94	F97	G98	Y99	G100	V101	Q102	T103	T104	G105	R106	S107	Q108										

- Molecule 4: Triplex gp44-b

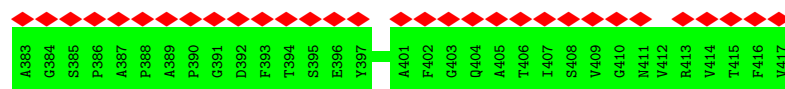
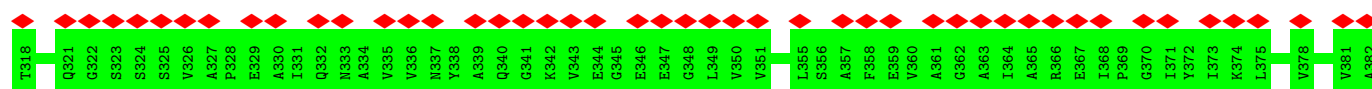
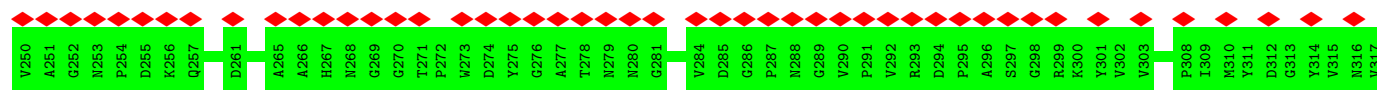
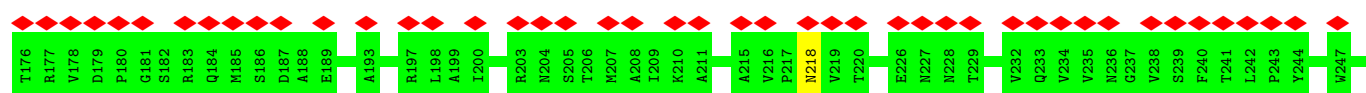
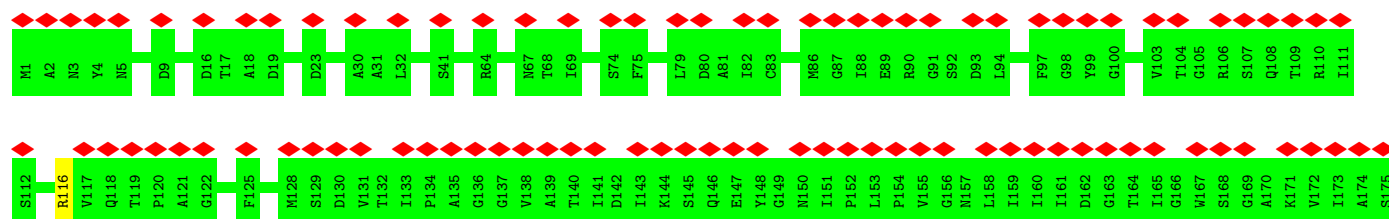


- Molecule 4: Triplex gp44-b

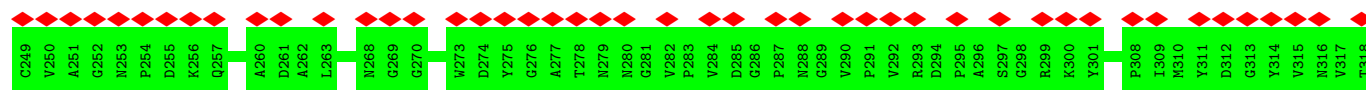
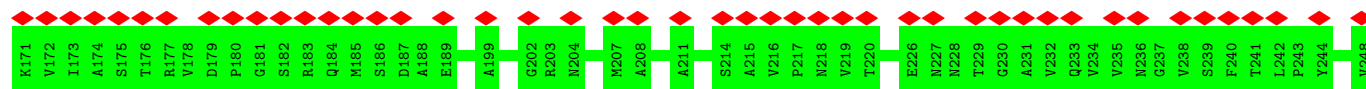
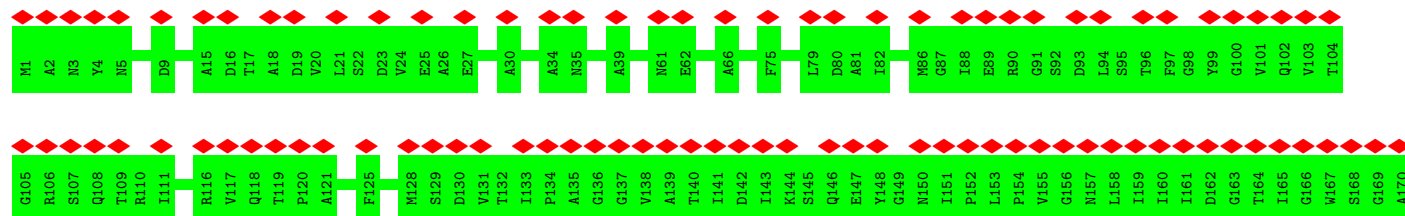




• Molecule 4: Triplex gp44-b



• Molecule 4: Triplex gp44-b

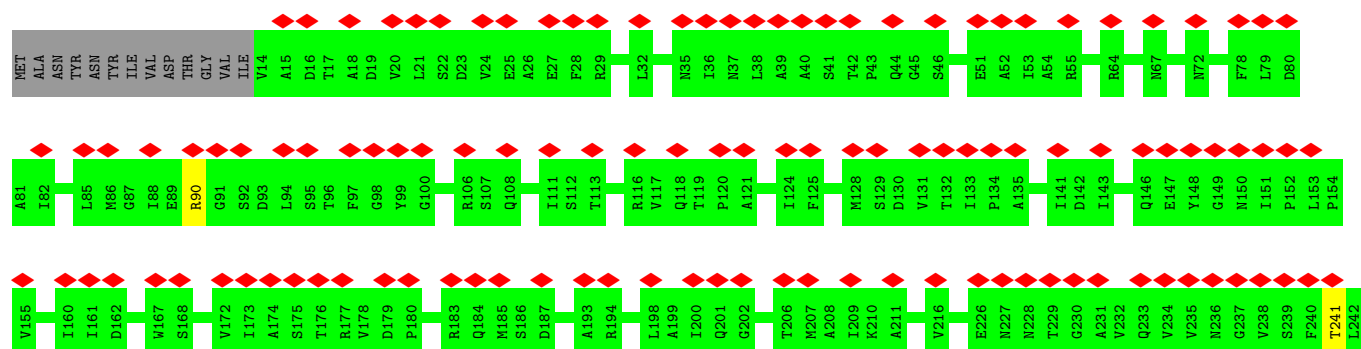


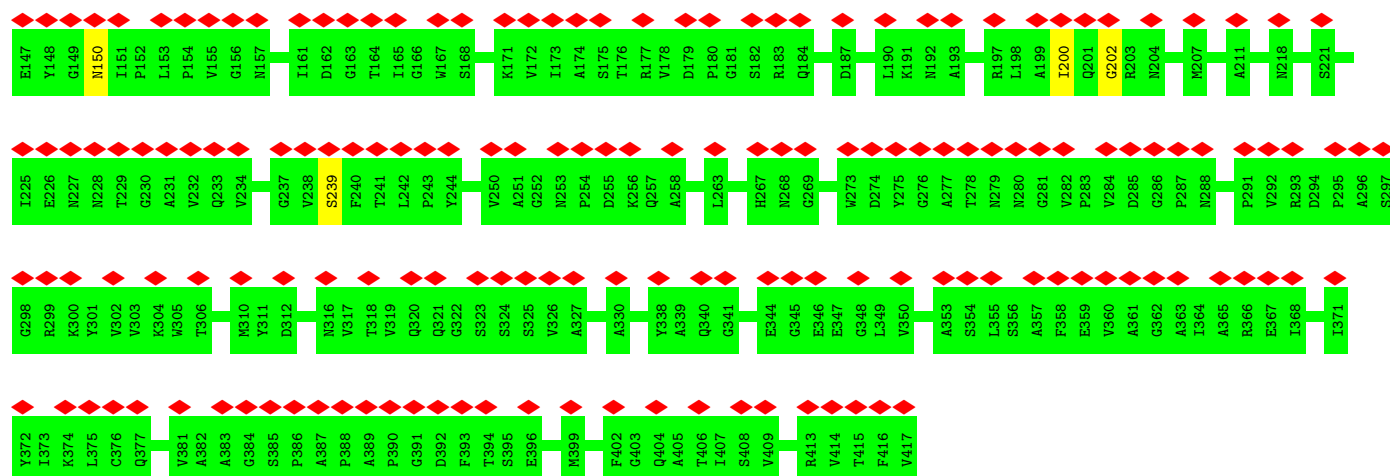


• Molecule 4: Triplex gp44-b

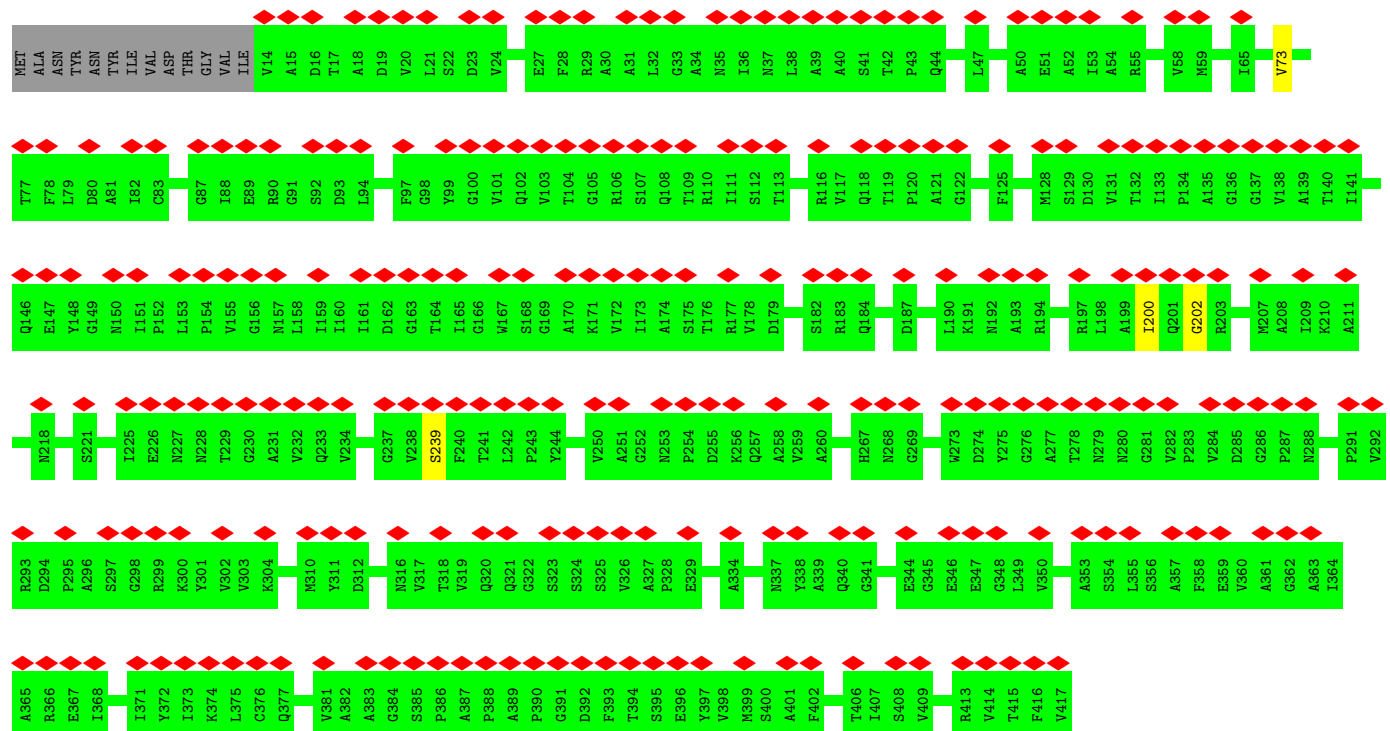


• Molecule 4: Triplex gp44-b

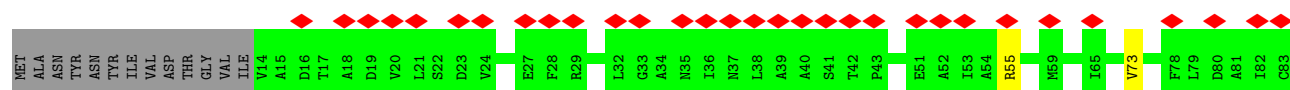


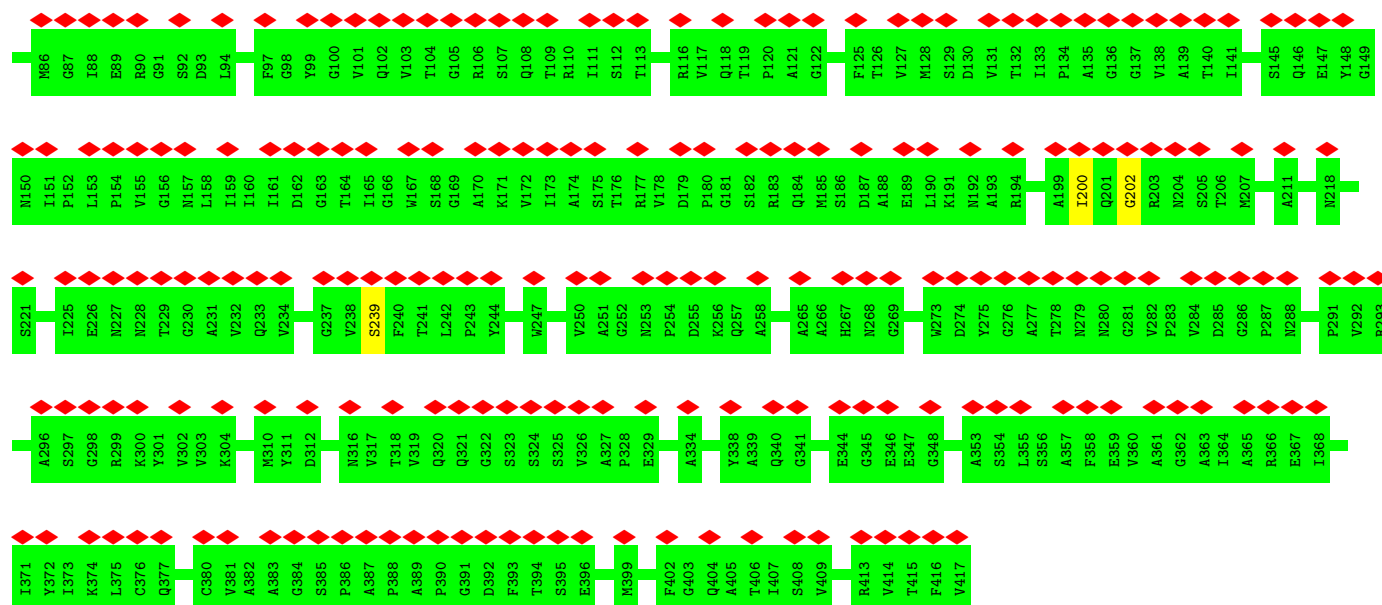


• Molecule 4: Triplex gp44-b

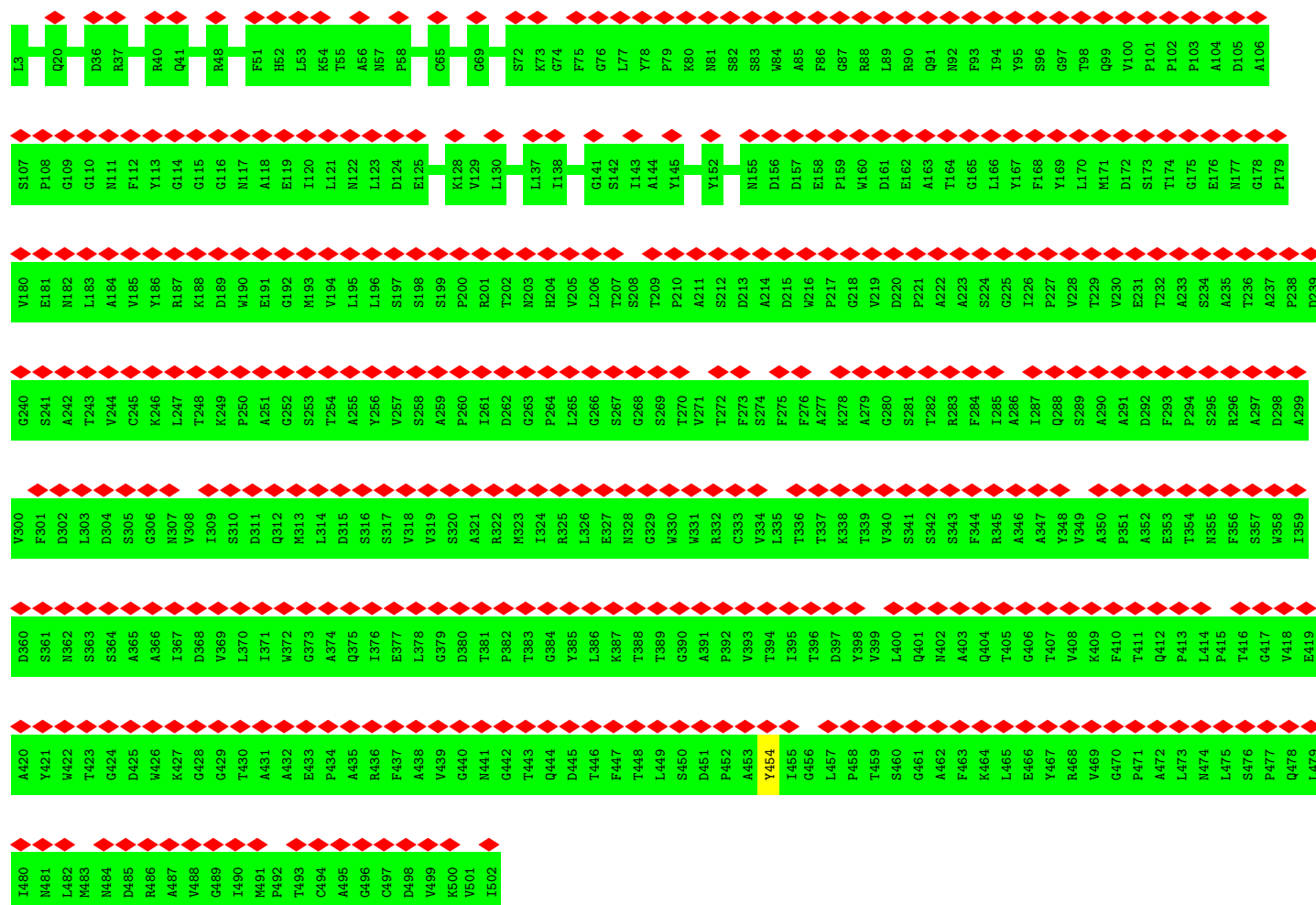
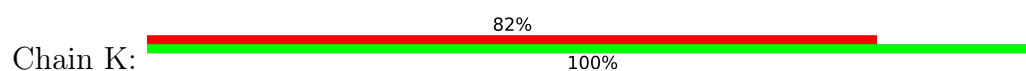


• Molecule 4: Triplex gp44-b

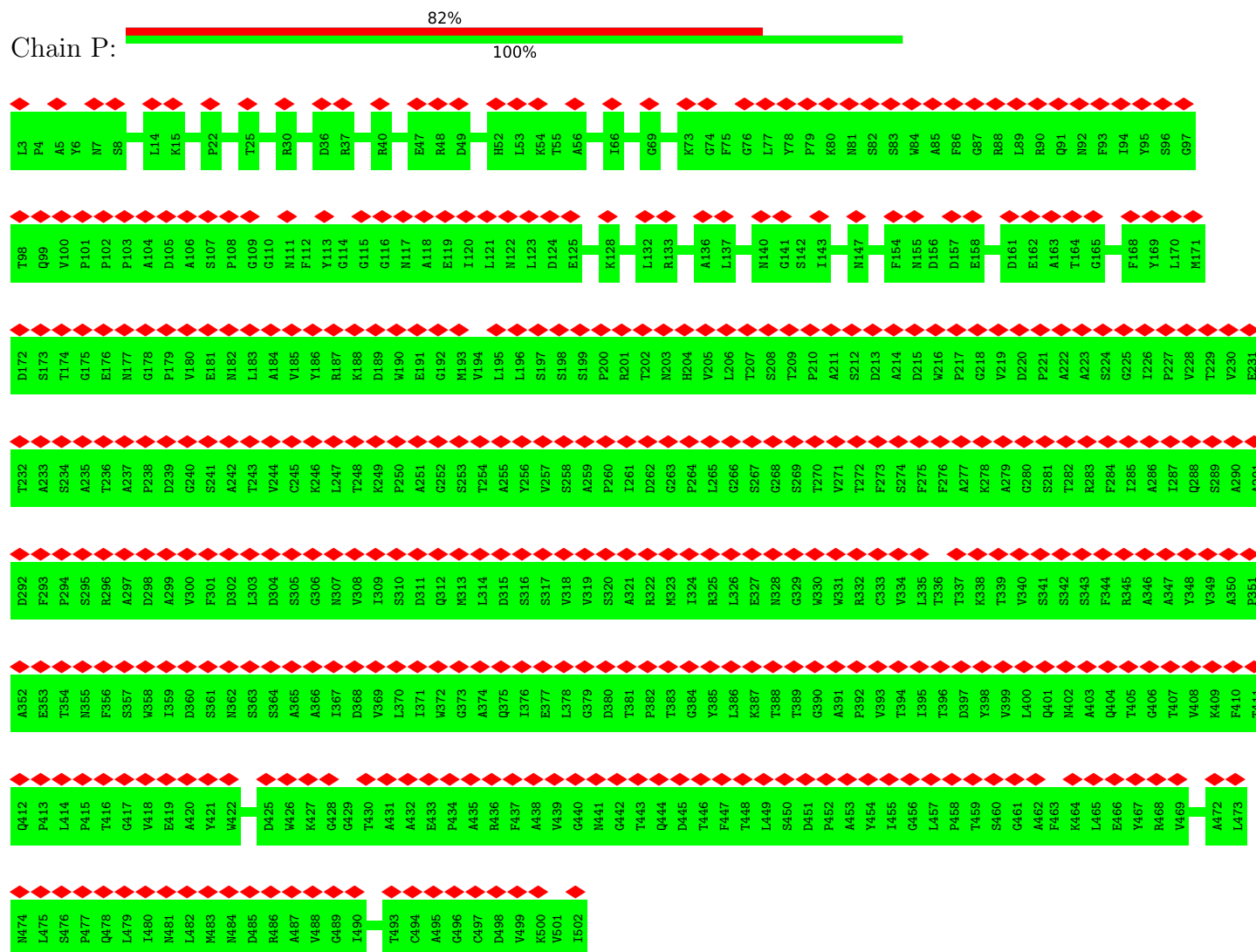




• Molecule 5: Triplex gp45

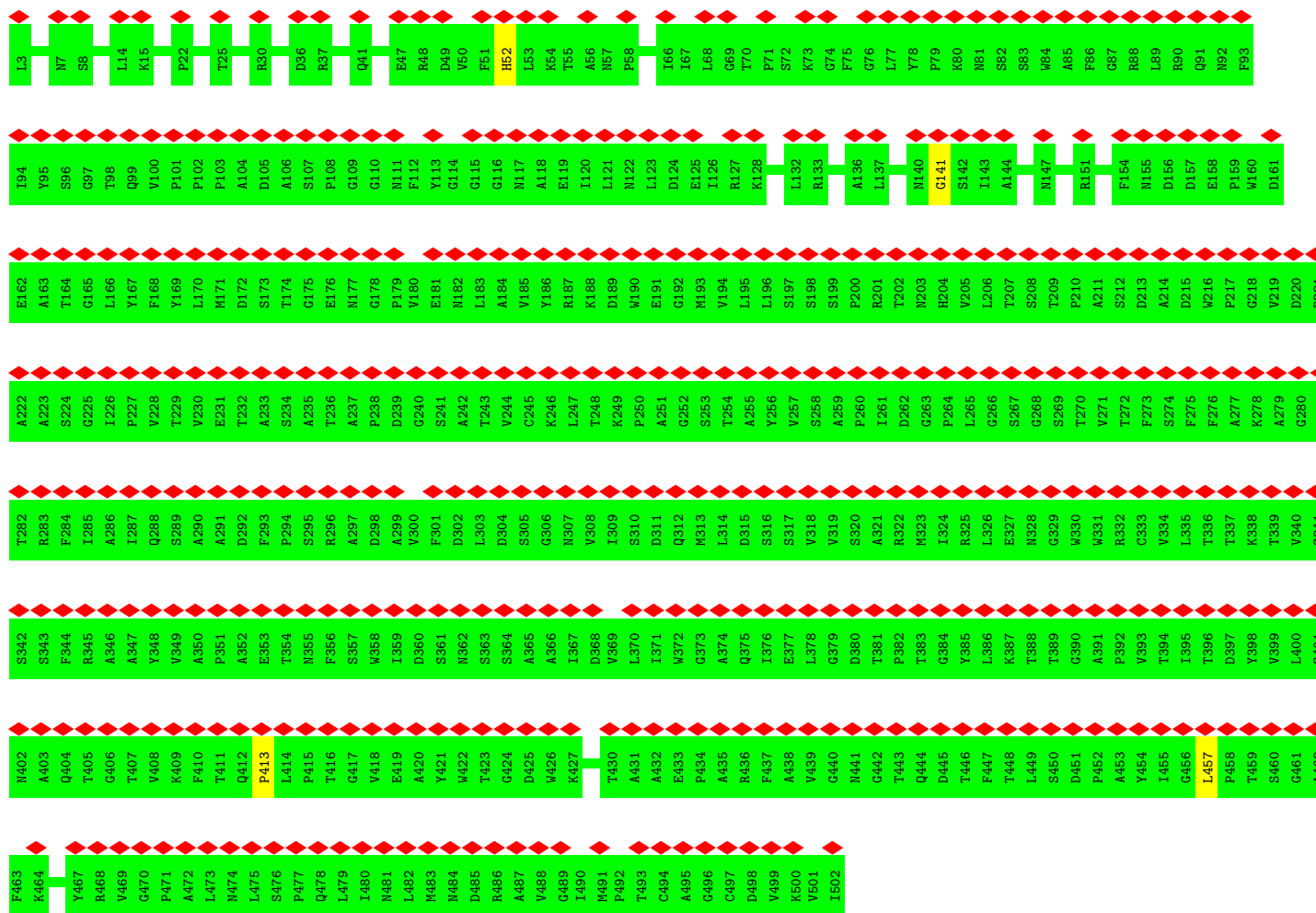
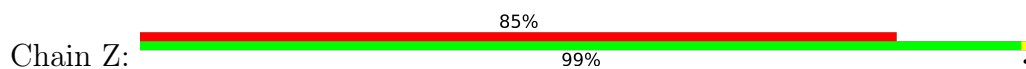


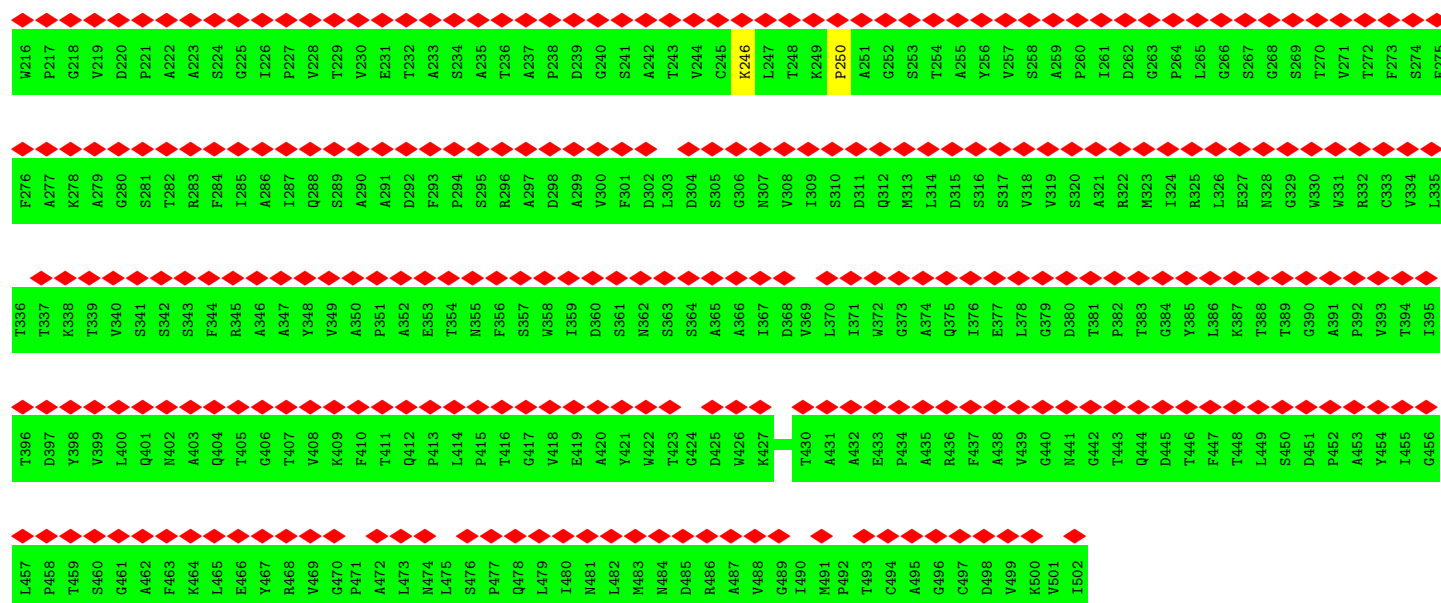
• Molecule 5: Triplex gp45



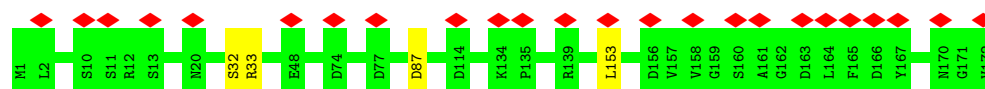


• Molecule 5: Triplex gp45

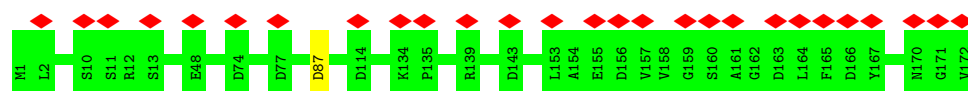




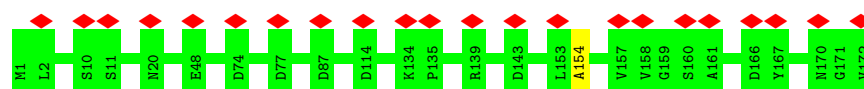
• Molecule 6: Baseplate component gp37



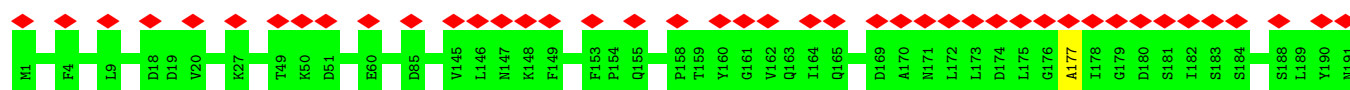
• Molecule 6: Baseplate component gp37



• Molecule 6: Baseplate component gp37

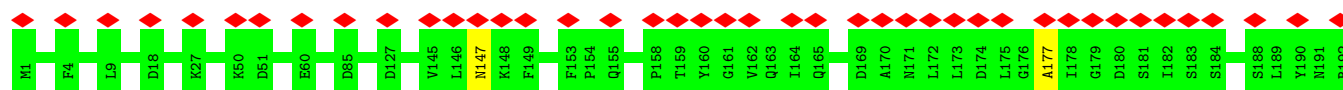


• Molecule 7: Baseplate component gp38

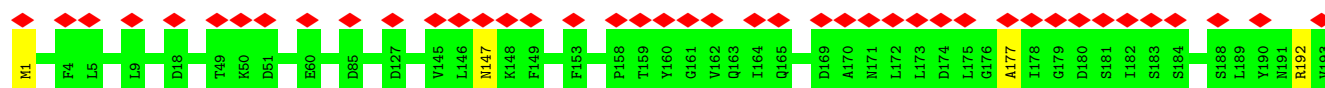




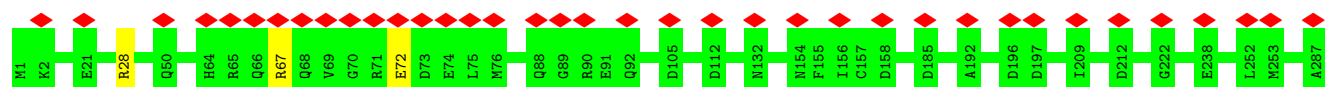
- Molecule 7: Baseplate component gp38



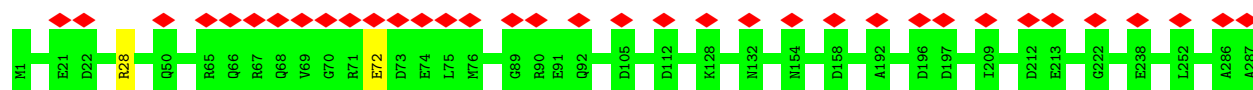
- Molecule 7: Baseplate component gp38



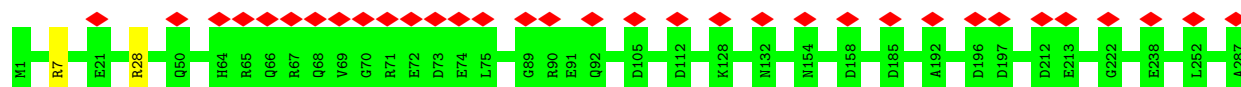
- Molecule 8: Baseplate hub gp41



- Molecule 8: Baseplate hub gp41

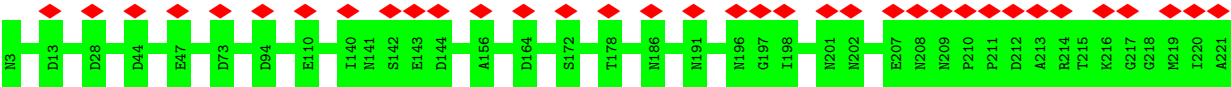


- Molecule 8: Baseplate hub gp41

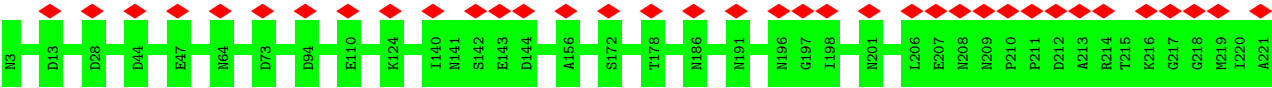


- Molecule 9: Baseplate spike gp43

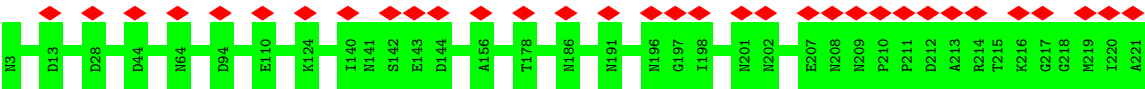




• Molecule 9: Baseplate spike gp43



• 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 (Å)	448.0, 448.0, 448.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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

All (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
3	X	49	TYR	CE2-CZ	40.72	1.91	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	49	TYR	CE1-CZ	39.03	1.89	1.38
3	N	146	TYR	CE1-CZ	30.77	1.78	1.38
3	N	146	TYR	CE2-CZ	30.66	1.78	1.38
3	X	49	TYR	CG-CD2	30.27	1.78	1.39
3	X	49	TYR	CG-CD1	29.20	1.77	1.39
3	N	146	TYR	CG-CD2	24.12	1.70	1.39
3	N	146	TYR	CG-CD1	23.07	1.69	1.39
5	Z	413	PRO	CG-CD	-13.35	1.06	1.50
6	A	32	SER	C-N	12.87	1.63	1.34
5	e	221	PRO	CG-CD	-12.67	1.08	1.50
6	A	33	ARG	N-CA	10.22	1.66	1.46
5	Z	413	PRO	N-CD	6.91	1.57	1.47
5	e	221	PRO	CB-CG	-5.31	1.23	1.50

All (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
5	Z	413	PRO	CA-N-CD	-11.79	94.99	111.50
5	e	221	PRO	CB-CG-CD	10.16	146.13	106.50
7	o	1	MET	CB-CG-SD	9.88	142.04	112.40
5	Z	413	PRO	CA-CB-CG	-8.57	87.71	104.00
6	A	33	ARG	CB-CA-C	-8.16	94.08	110.40
6	A	33	ARG	N-CA-CB	7.63	124.33	110.60
5	j	250	PRO	N-CD-CG	-6.90	92.85	103.20
5	e	221	PRO	CA-N-CD	-6.16	102.88	111.50
5	Z	457	LEU	CA-CB-CG	6.00	129.11	115.30
6	A	32	SER	CA-C-O	-5.69	108.15	120.10
3	X	49	TYR	CZ-CE2-CD2	-5.65	114.72	119.80
3	X	49	TYR	CB-CG-CD1	-5.45	117.73	121.00
7	o	1	MET	CA-CB-CG	5.23	122.19	113.30
6	A	33	ARG	CA-CB-CG	5.23	124.90	113.40
5	Z	141	GLY	N-CA-C	5.20	126.10	113.10

There are no chirality outliers.

All (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
1	f	65	ARG	Peptide
4	t	200	ILE	Peptide
4	u	200	ILE	Peptide
4	v	200	ILE	Peptide
4	v	55	ARG	Sidechain

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
6	B	87	ASP
4	t	239	SER
4	u	239	SER
4	v	239	SER
3	I	89	PHE
7	k	147	ASN
7	o	147	ASN
4	t	73	VAL
4	t	202	GLY
4	u	73	VAL
4	u	202	GLY
4	v	202	GLY
4	v	73	VAL
8	l	72	GLU
3	I	96	ILE
3	S	96	ILE
2	b	42	ARG
3	h	96	ILE
7	D	177	ALA
2	H	42	ARG
5	K	454	TYR
2	M	42	ARG
2	g	92	ILE
6	C	154	ALA

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Mol	Chain	Res	Type
8	E	72	GLU
7	k	177	ALA
7	o	177	ALA
4	q	241	THR
4	r	241	THR
4	s	241	THR
2	H	92	ILE
2	H	94	ILE
2	M	92	ILE
2	W	92	ILE
2	R	94	ILE
2	M	94	ILE
2	R	92	ILE
2	b	92	ILE
2	g	94	ILE
2	W	28	VAL

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	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	65	ARG
4	J	228	ASN
4	J	293	ARG
4	O	106	ARG
1	V	50	ARG
4	Y	106	ARG
4	Y	203	ARG
4	Y	228	ASN
4	Y	413	ARG
5	Z	52	HIS
3	c	150	GLN
4	d	116	ARG
4	d	218	ASN
4	i	411	ASN
5	j	246	LYS
8	E	28	ARG
8	E	67	ARG
8	l	28	ARG
8	m	7	ARG
8	m	28	ARG
7	o	192	ARG
4	q	413	ARG
4	r	90	ARG
4	t	150	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	35	ASN
2	H	33	GLN
2	H	109	HIS
4	J	268	ASN
4	J	332	GLN
2	M	33	GLN
1	Q	35	ASN
4	T	35	ASN
4	T	228	ASN
4	T	268	ASN
5	U	402	ASN
1	V	30	ASN
4	Y	108	GLN
4	Y	228	ASN
1	a	35	ASN
1	a	59	GLN
2	b	109	HIS
3	c	150	GLN
4	d	218	ASN
4	d	228	ASN
4	d	340	GLN
1	f	35	ASN
2	g	109	HIS
3	h	116	ASN
7	D	10	ASN
7	D	191	ASN
8	E	64	HIS
9	F	92	GLN
9	n	53	GLN
9	n	92	GLN
9	n	203	HIS
9	p	92	GLN
9	p	203	HIS
4	r	268	ASN
4	s	268	ASN
4	t	150	ASN
4	t	157	ASN
4	u	150	ASN
4	u	157	ASN
4	u	201	GLN
4	u	288	ASN
4	u	316	ASN
4	v	157	ASN

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Mol	Chain	Res	Type
4	v	196	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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	32:SER	C	33:ARG	N	1.63

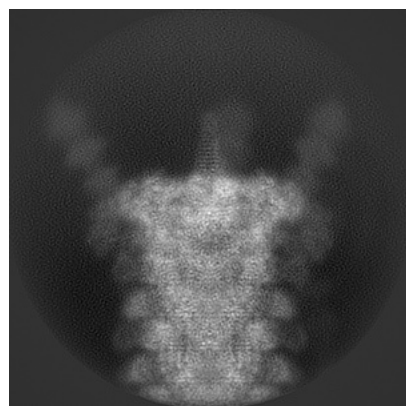
6 Map visualisation [i](#)

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.

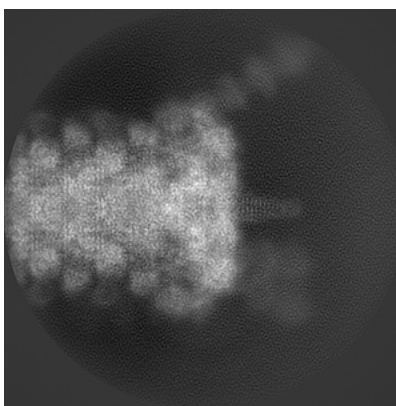
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

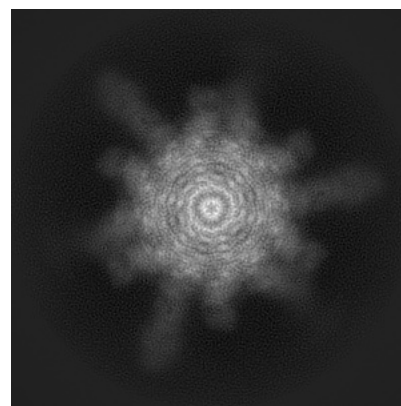
6.1.1 Primary map



X

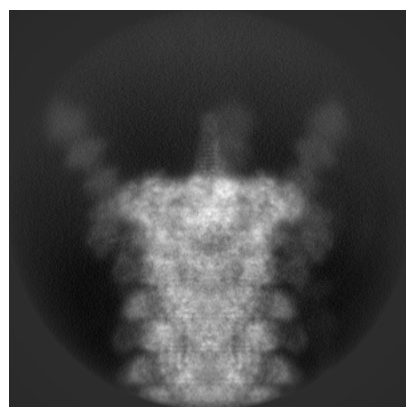


Y

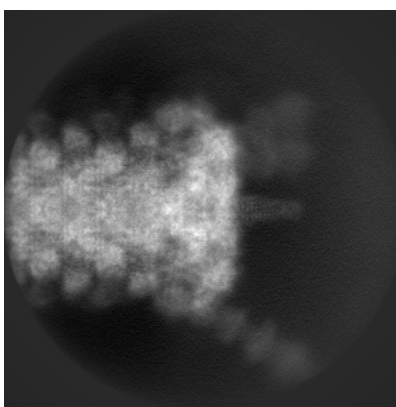


Z

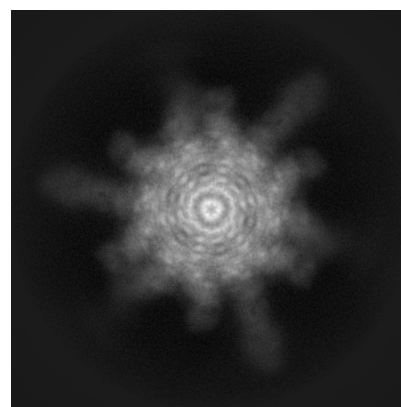
6.1.2 Raw map



X



Y

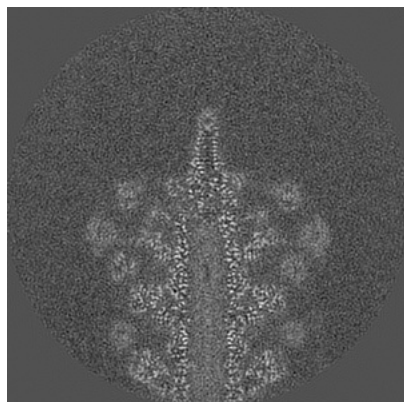


Z

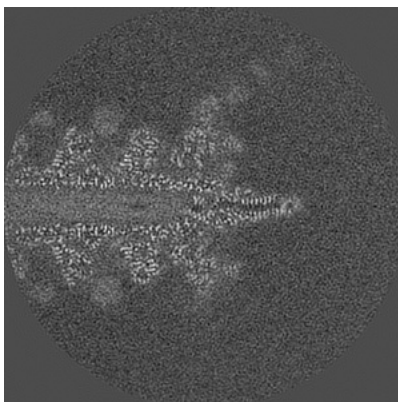
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

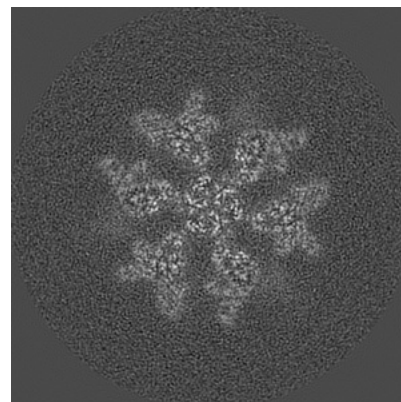
6.2.1 Primary map



X Index: 200

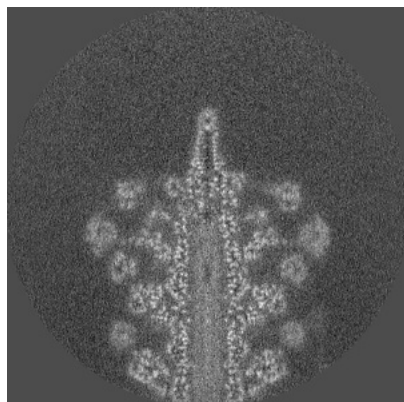


Y Index: 200

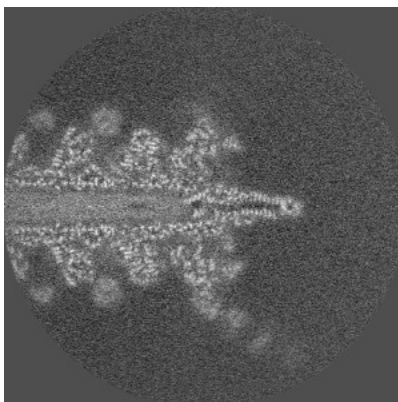


Z Index: 200

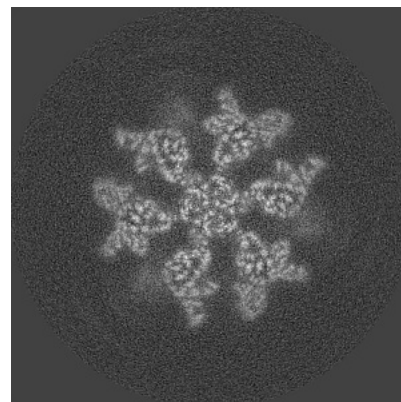
6.2.2 Raw map



X Index: 200



Y Index: 200

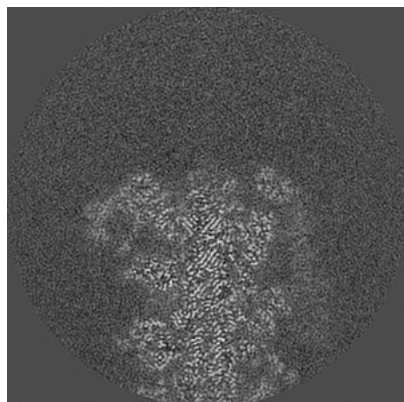


Z Index: 200

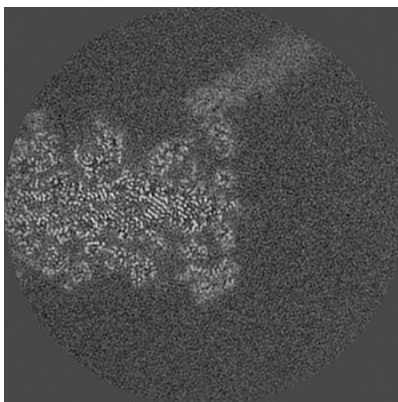
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

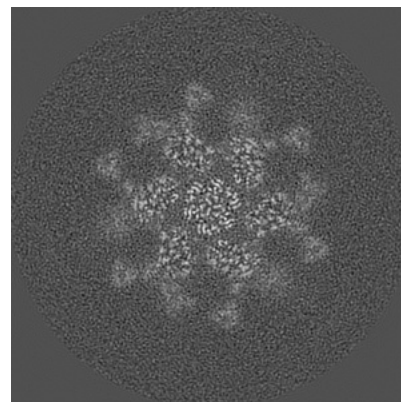
6.3.1 Primary map



X Index: 220

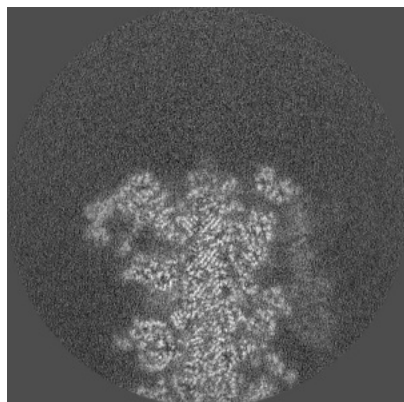


Y Index: 219

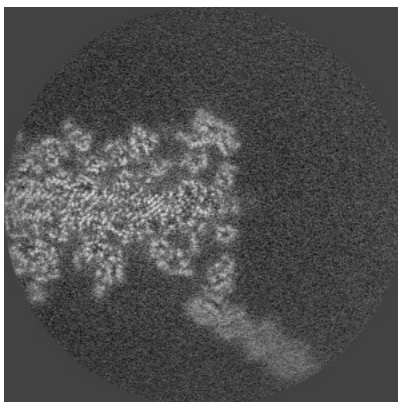


Z Index: 191

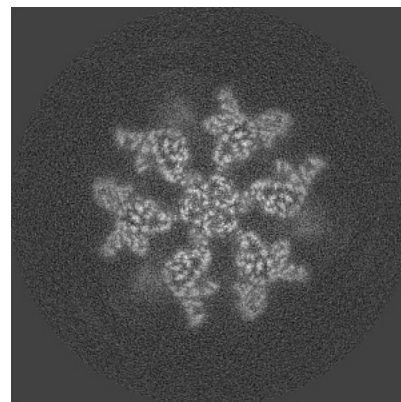
6.3.2 Raw map



X Index: 180



Y Index: 220

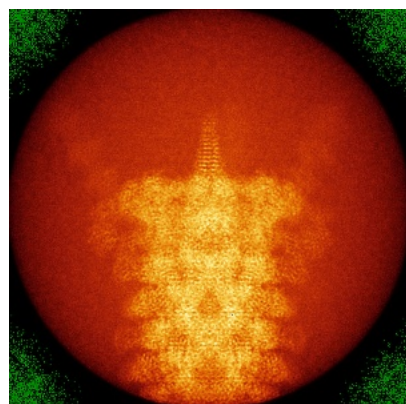


Z Index: 200

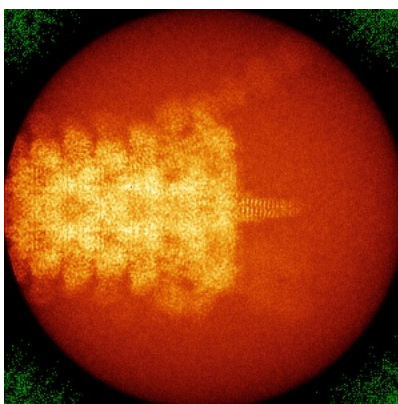
The images above show the largest variance slices of the map in three orthogonal directions.

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

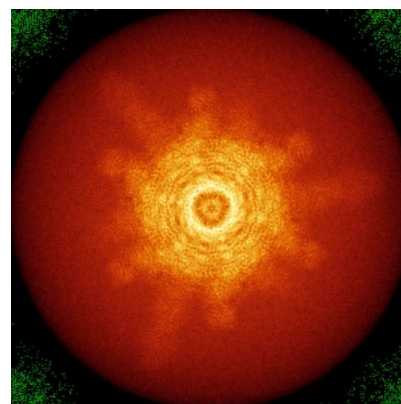
6.4.1 Primary map



X

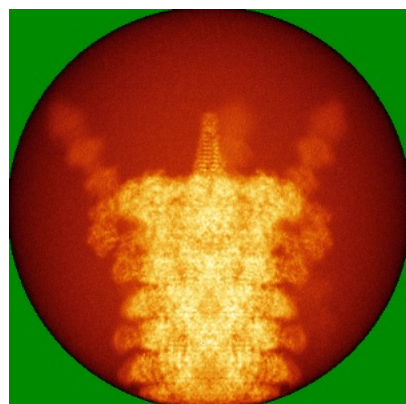


Y

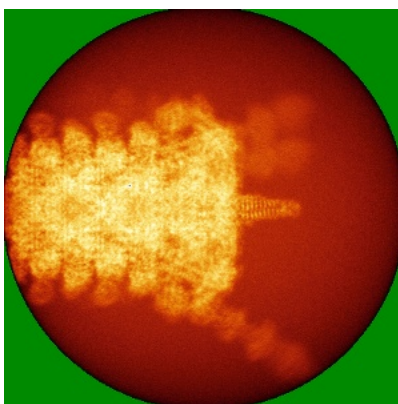


Z

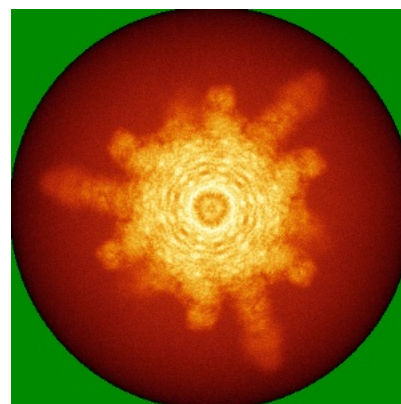
6.4.2 Raw map



X



Y

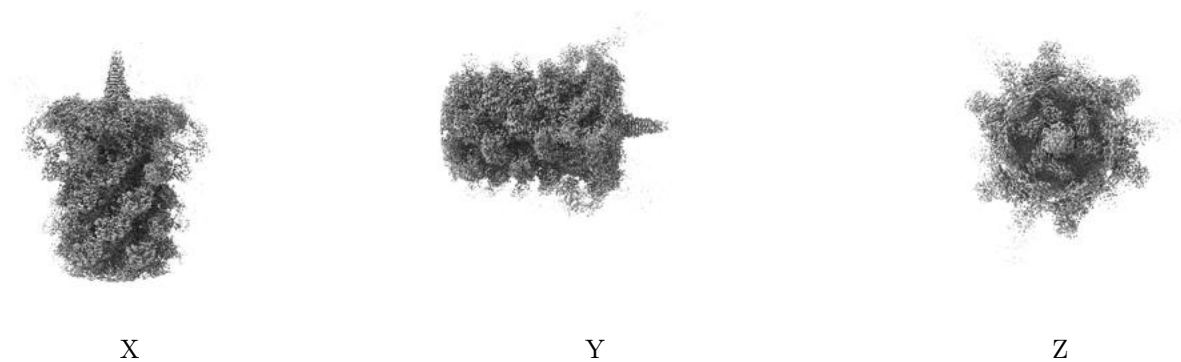


Z

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.

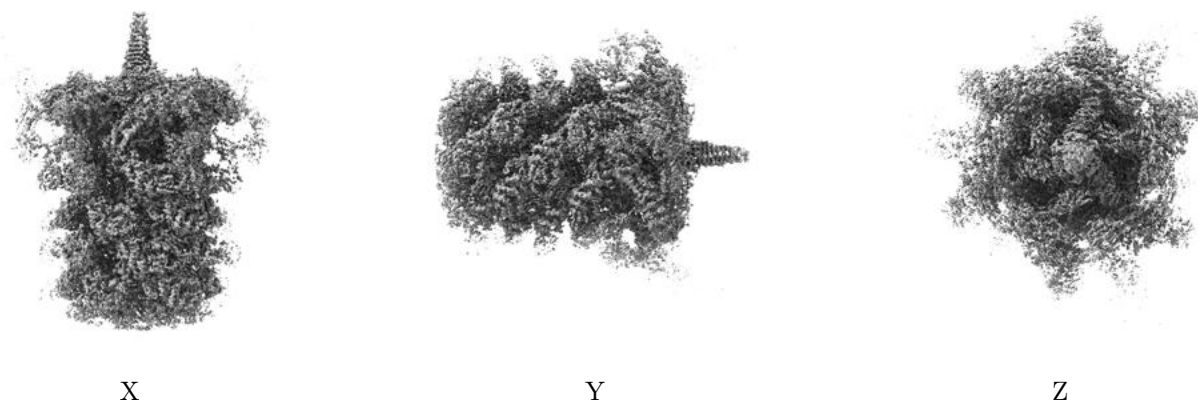
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

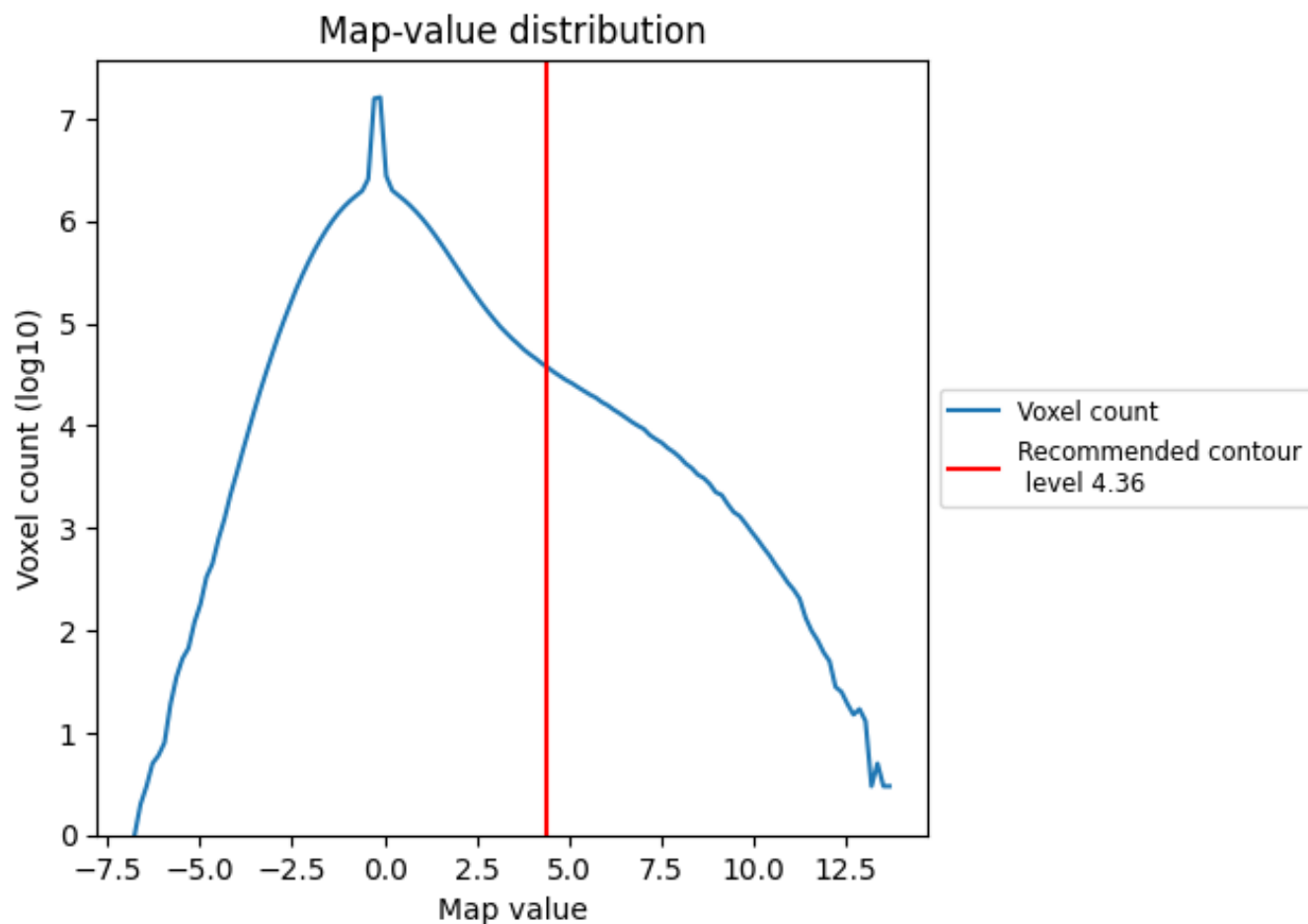
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

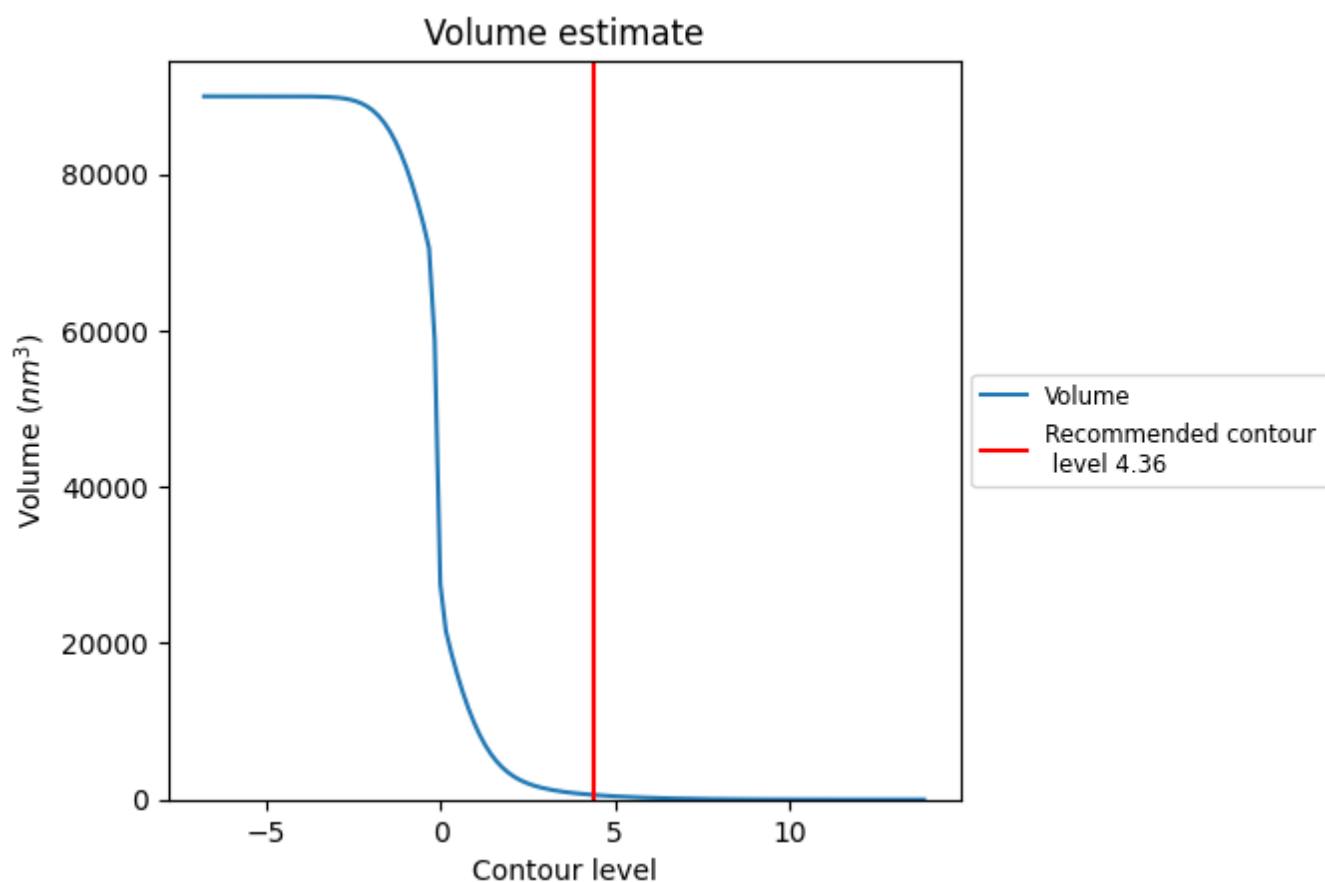
This section contains the results of statistical analysis of the map.

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.

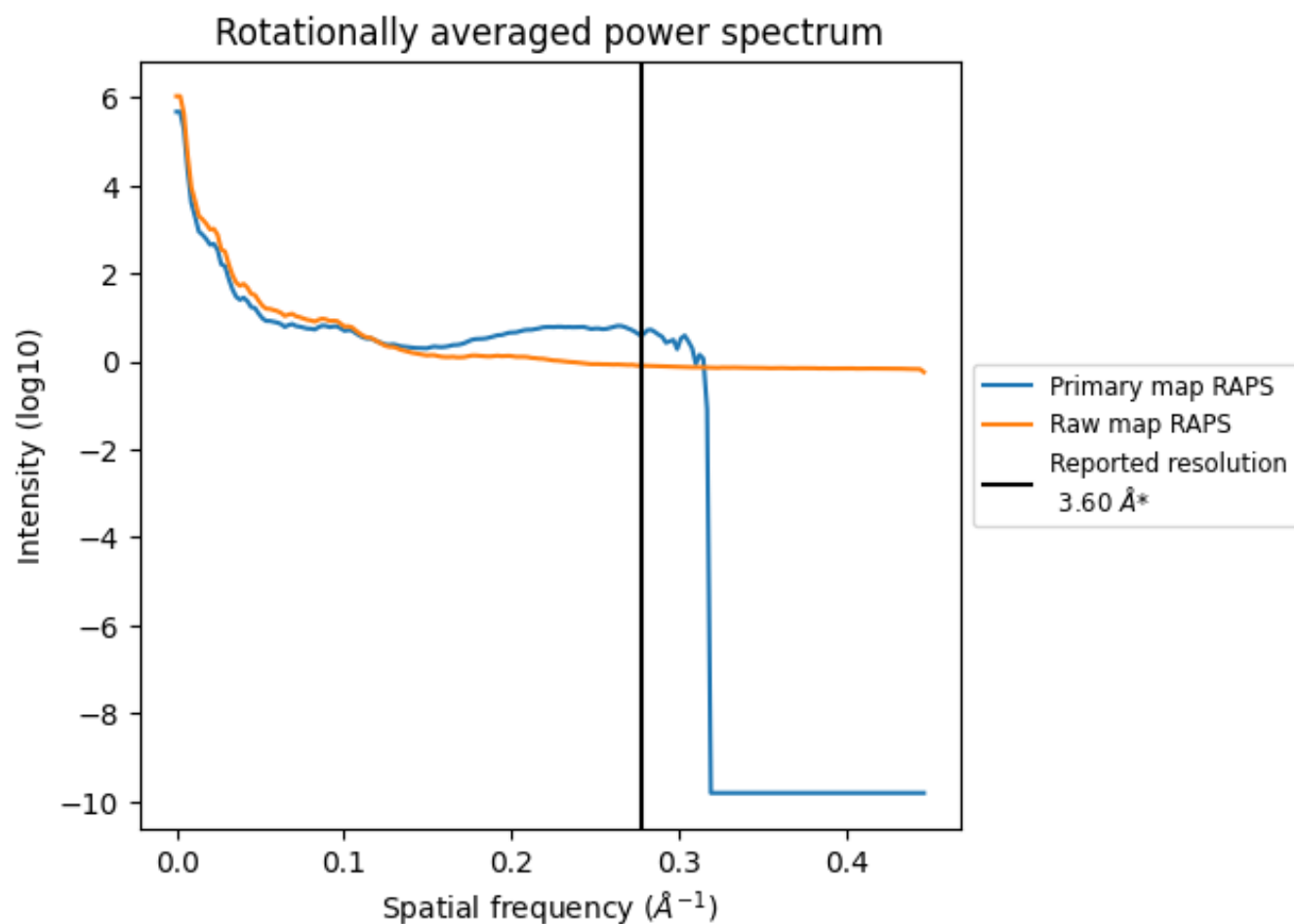
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 602 nm³; 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 ⓘ

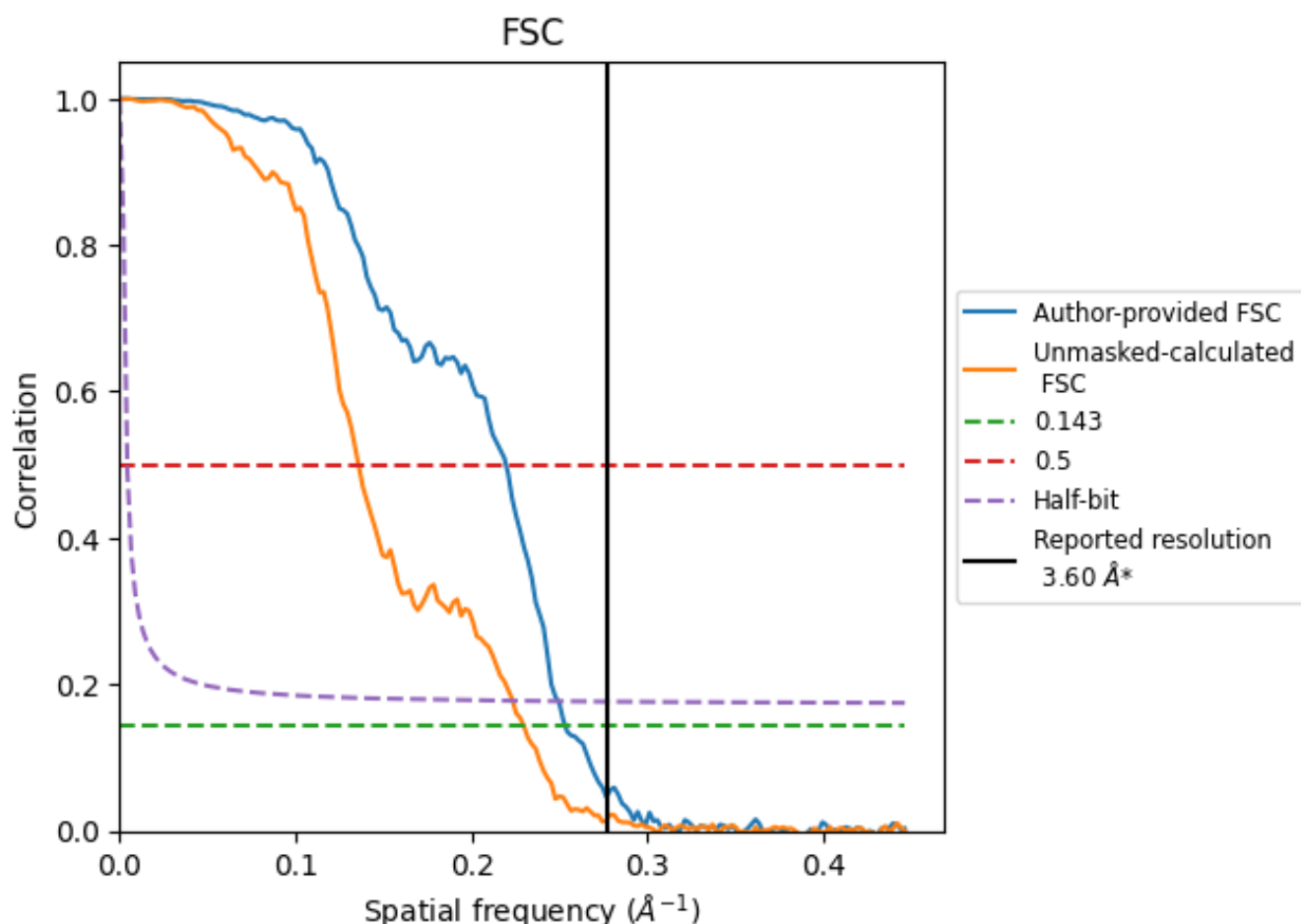


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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](#)

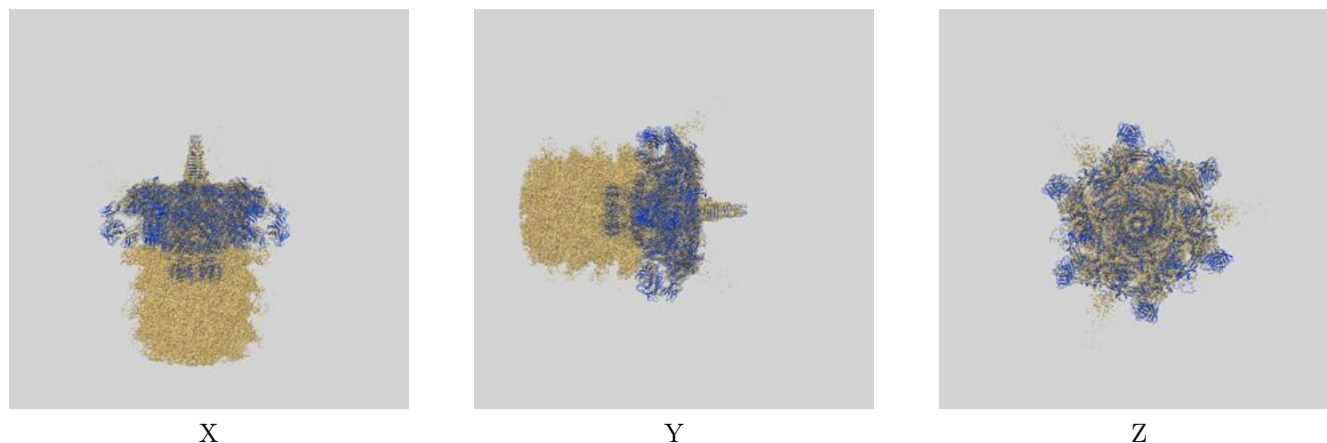
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.95	4.55	4.01
Unmasked-calculated*	4.35	7.36	4.47

*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](#)

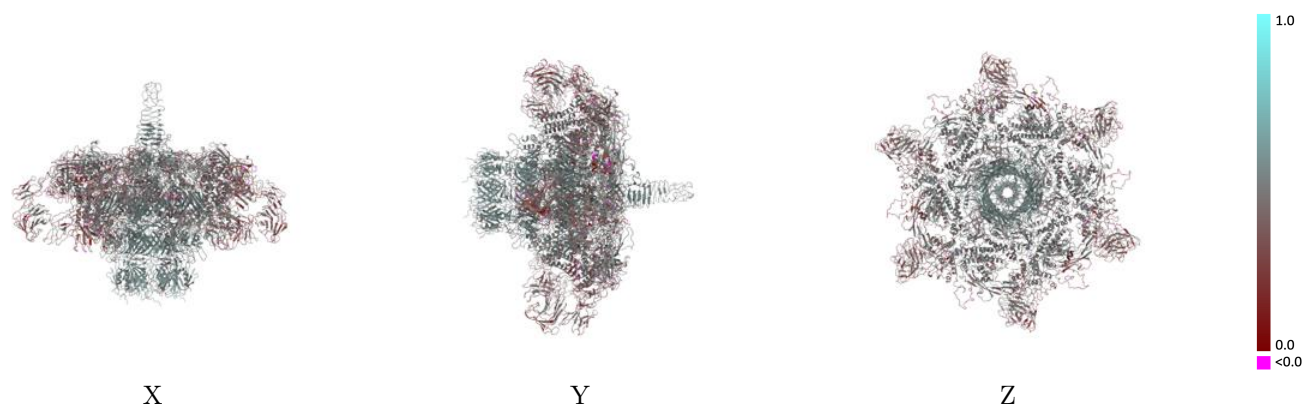
This section contains information regarding the fit between EMDB map EMD-28405 and PDB model 8EON. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



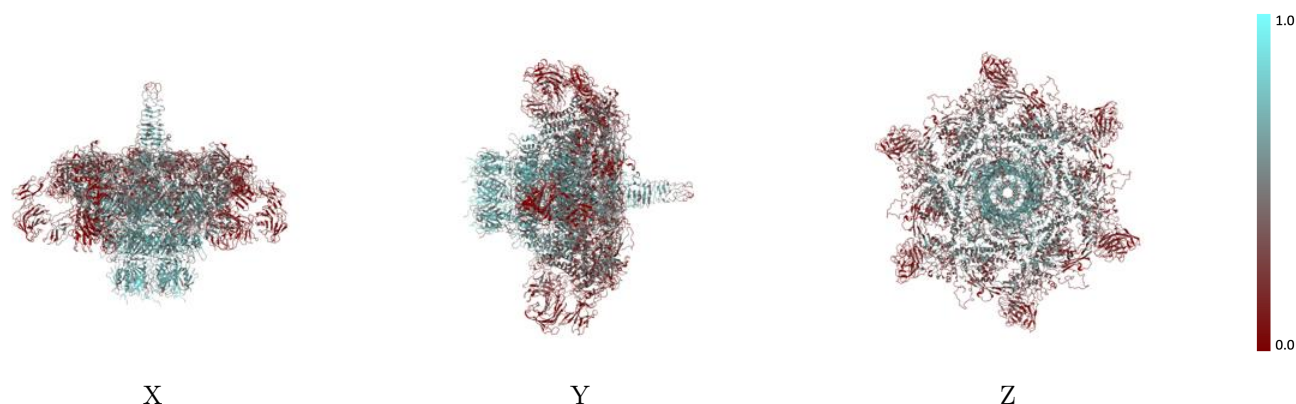
The images above show the 3D surface view of the map at the recommended contour level 4.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



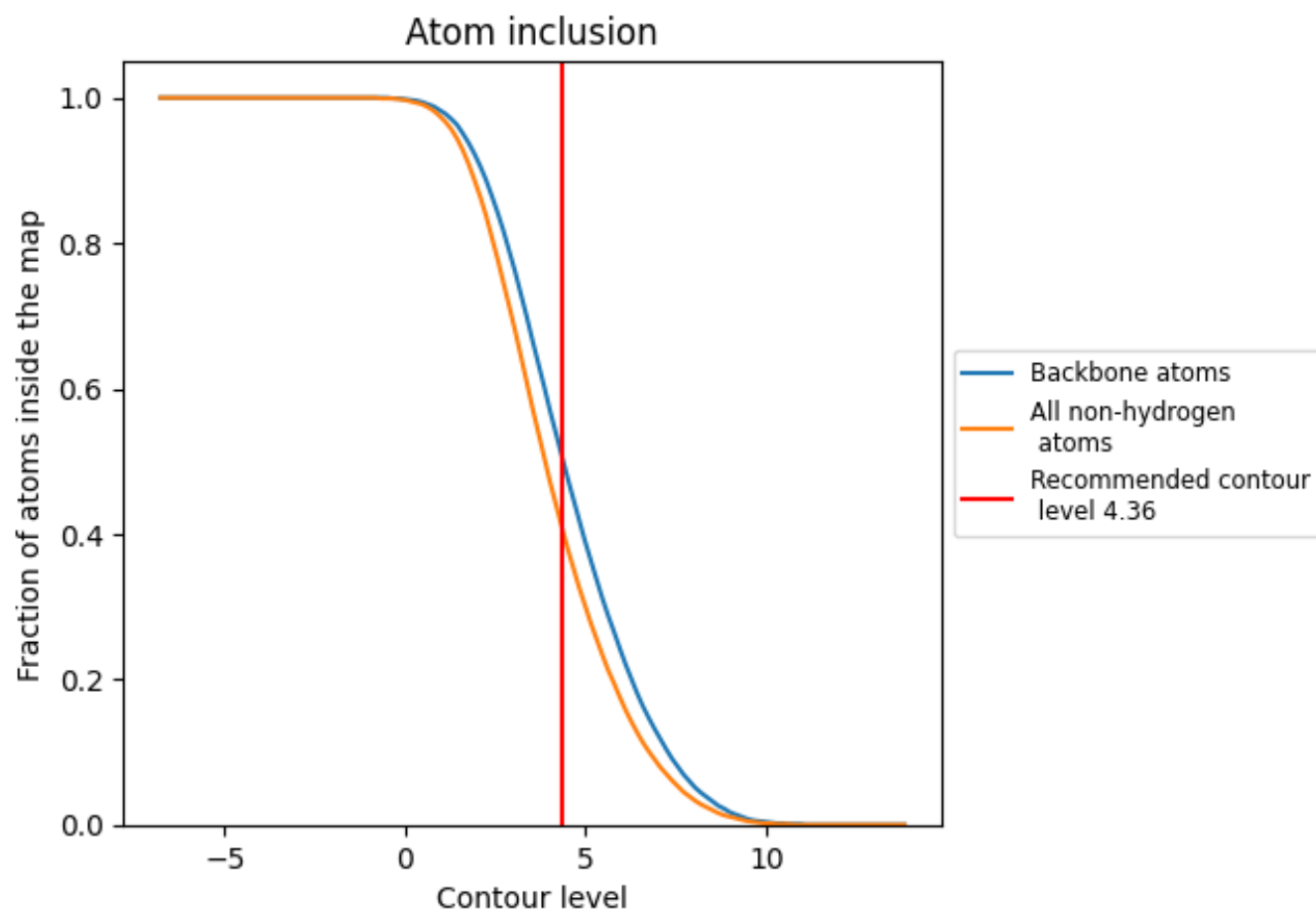
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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