



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 11:32 AM JST

PDB ID : 7FJ1
EMDB ID : EMD-31611
Title : Cryo-EM structure of pseudorabies virus C-capsid
Authors : Zheng, Q.; Li, S.; Zha, Z.; Sun, H.
Deposited on : 2021-08-02
Resolution : 4.43 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

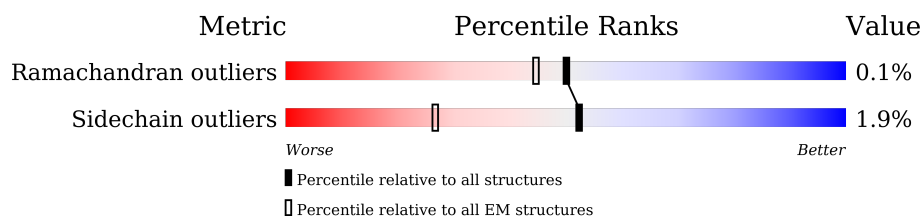
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.43 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	207382	16835
Sidechain outliers	206894	16415

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	0	1330	<div> <div>27%</div> <div>98%</div> </div>
1	A	1330	<div> <div>22%</div> <div>98%</div> </div>
1	S	1330	<div> <div>27%</div> <div>97%</div> </div>
1	U	1330	<div> <div>23%</div> <div>98%</div> </div>
1	a	1330	<div> <div>27%</div> <div>97%</div> </div>
1	e	1330	<div> <div>35%</div> <div>85%</div> <div>15%</div> </div>
1	f	1330	<div> <div>23%</div> <div>98%</div> </div>
1	g	1330	<div> <div>26%</div> <div>98%</div> </div>
1	l	1330	<div> <div>25%</div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain	
1	m	1330	25%	98%
1	n	1330	27%	98%
1	p	1330	25%	98%
1	q	1330	27%	98%
1	u	1330	22%	98%
1	w	1330	27%	98%
1	y	1330	23%	98%
2	1	296	26%	94%
2	2	296	27%	93%
2	3	296	30%	94%
2	j	296	53%	90%
2	k	296	50%	94%
2	o	296	29%	100%
2	s	296	25%	94%
2	v	296	29%	97%
2	x	296	36%	100%
2	z	296	34%	99%
3	B	597	72%	87%
4	E	103	11%	78%
4	F	103	16%	78%
4	G	103	21%	78%
4	H	103	10%	78%
4	I	103	21%	78%
4	J	103	14%	76%
4	K	103	10%	77%

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Mol	Chain	Length	Quality of chain
4	L	103	
4	M	103	
4	N	103	
4	O	103	
4	P	103	
4	Q	103	
4	R	103	
4	V	103	
5	T	368	
5	h	368	
5	i	368	
5	r	368	
5	t	368	
6	X	534	
6	c	534	
7	Y	62	
7	Z	62	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 210927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	A	1308	Total	C	N	O	S	0	0
			10112	6393	1820	1837	62		
1	S	1289	Total	C	N	O	S	0	0
			9975	6307	1797	1812	59		
1	U	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	a	1289	Total	C	N	O	S	0	0
			9974	6311	1797	1805	61		
1	e	1126	Total	C	N	O	S	0	0
			8722	5528	1561	1579	54		
1	f	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	g	1310	Total	C	N	O	S	0	0
			10125	6401	1823	1840	61		
1	l	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	m	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	n	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	p	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	q	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	u	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	w	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	y	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		

- Molecule 2 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	2	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	3	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	j	267	Total	C	N	O	S	0	0
			2009	1269	365	364	11		
2	k	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	o	296	Total	C	N	O	S	0	0
			2229	1403	414	401	11		
2	s	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	v	289	Total	C	N	O	S	0	0
			2189	1380	404	394	11		
2	x	296	Total	C	N	O	S	0	0
			2229	1403	414	401	11		
2	z	294	Total	C	N	O	S	0	0
			2210	1391	412	396	11		

- Molecule 3 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	524	Total	C	N	O	S	0	0
			4023	2540	764	706	13		

- Molecule 4 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	F	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	G	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	H	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	I	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	J	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	K	91	Total	C	N	O	S	0	0
			722	453	139	128	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	M	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	N	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	O	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	P	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	Q	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	R	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	V	91	Total	C	N	O	S	0	0
			722	453	139	128	2		

- Molecule 5 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	h	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	i	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	r	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	t	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		

- Molecule 6 is a protein called DNA packaging tegument protein UL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	73	Total	C	N	O	S	0	0
			552	346	109	96	1		
6	c	75	Total	C	N	O	S	0	0
			558	350	111	96	1		

- Molecule 7 is a protein called VP1/2.

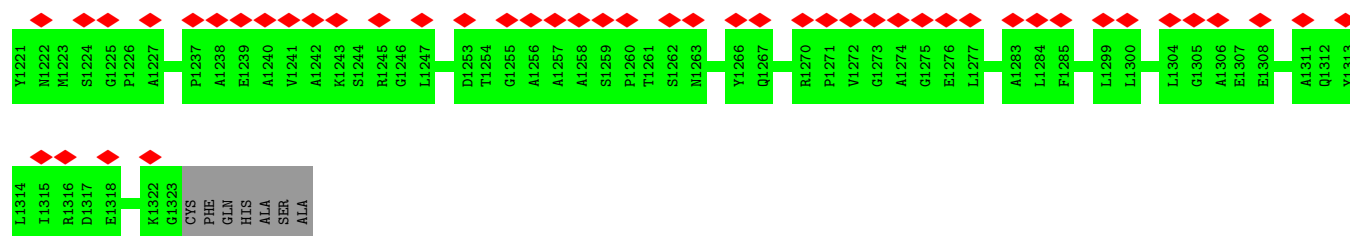
Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	45	Total	C	N	O	S	0	0
			353	224	72	56	1		
7	Z	35	Total	C	N	O	S	0	0
			288	180	62	45	1		

3 Residue-property plots

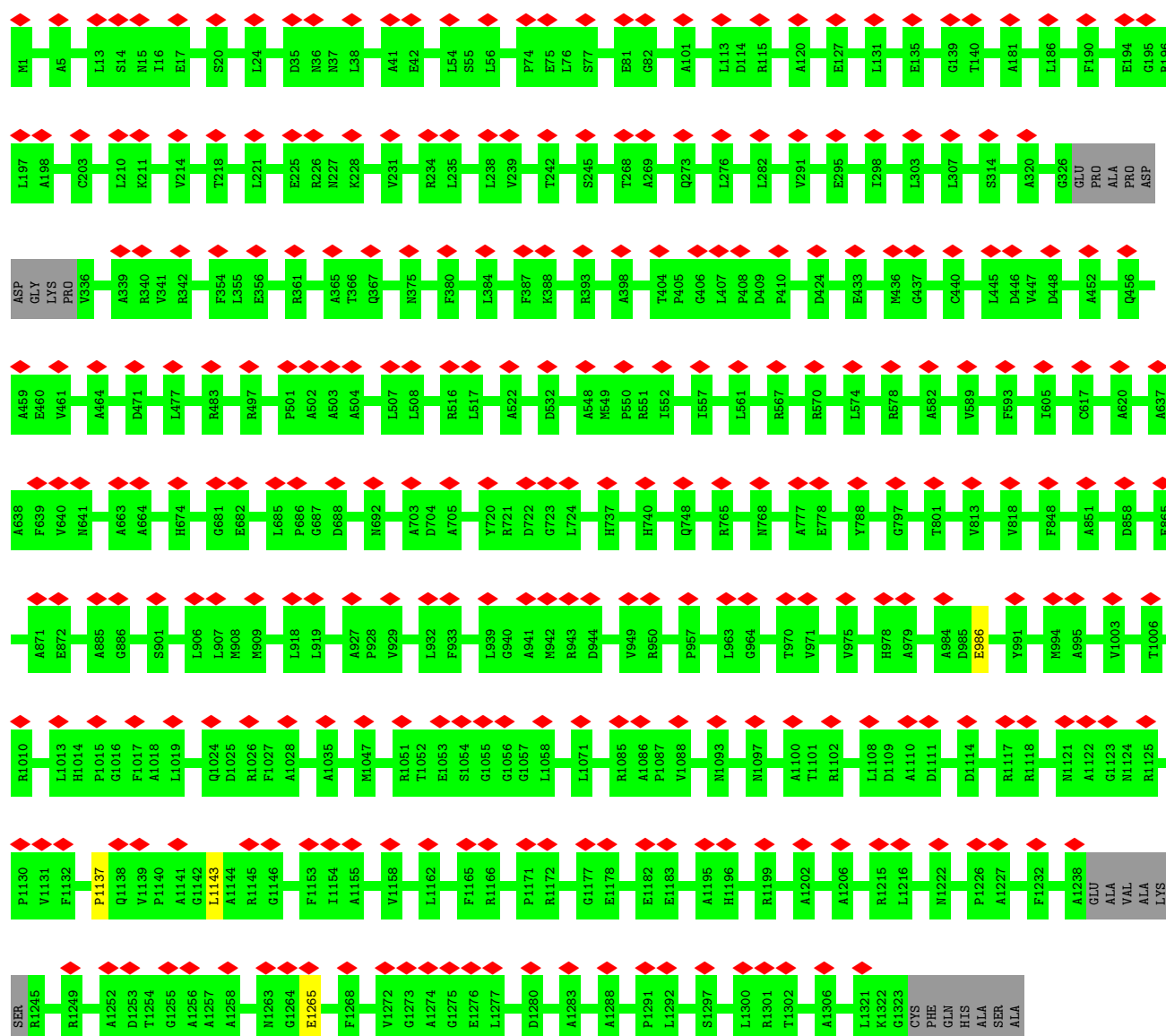
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Major capsid protein





• Molecule 1: Major capsid protein

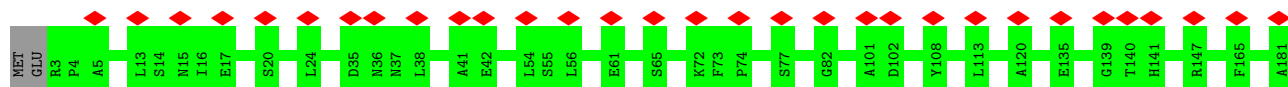


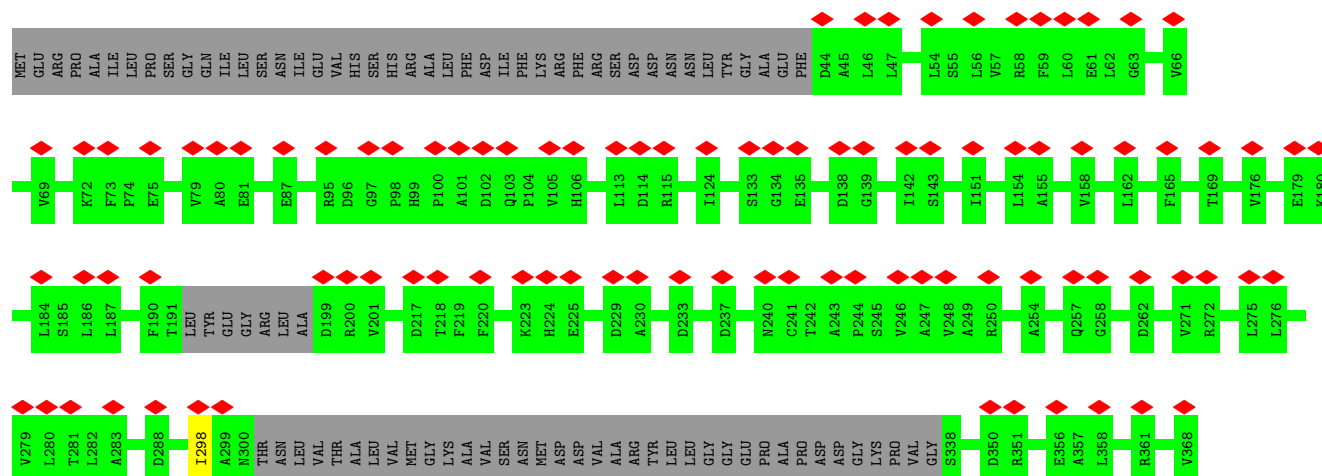
• Molecule 1: Major capsid protein

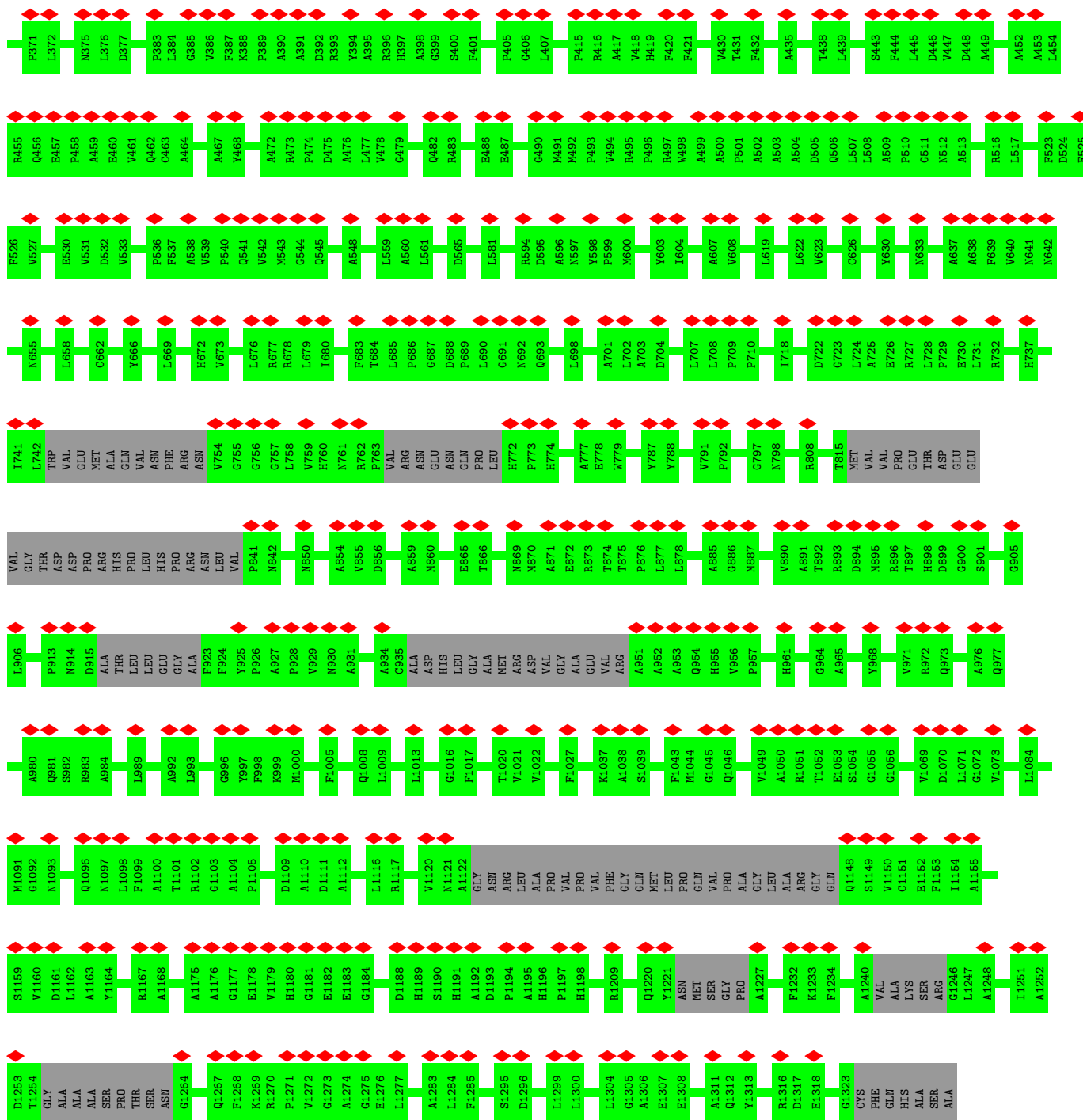




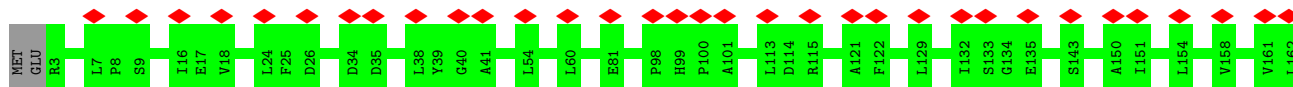
• Molecule 1: Major capsid protein





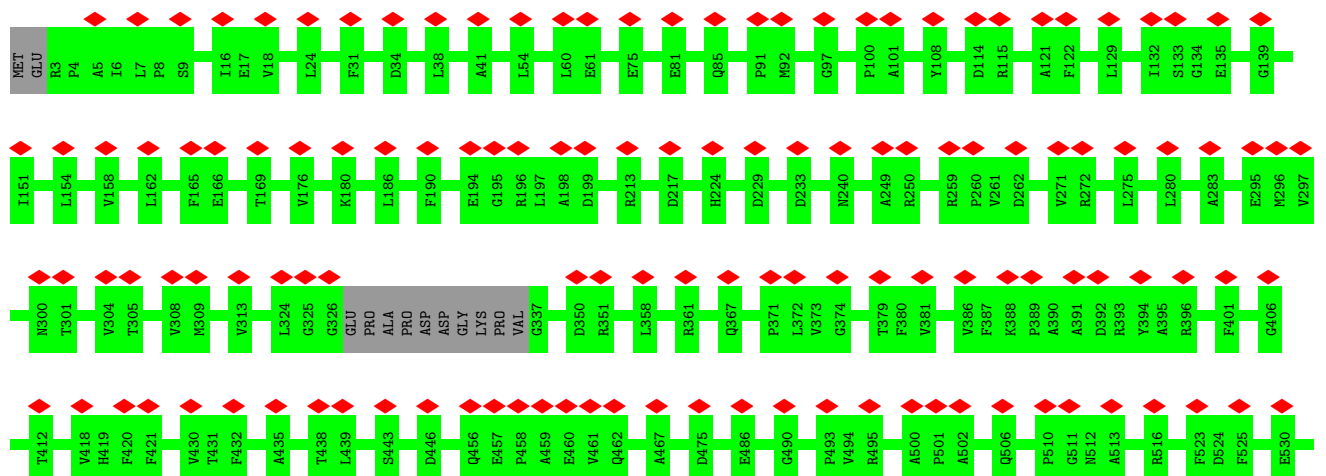


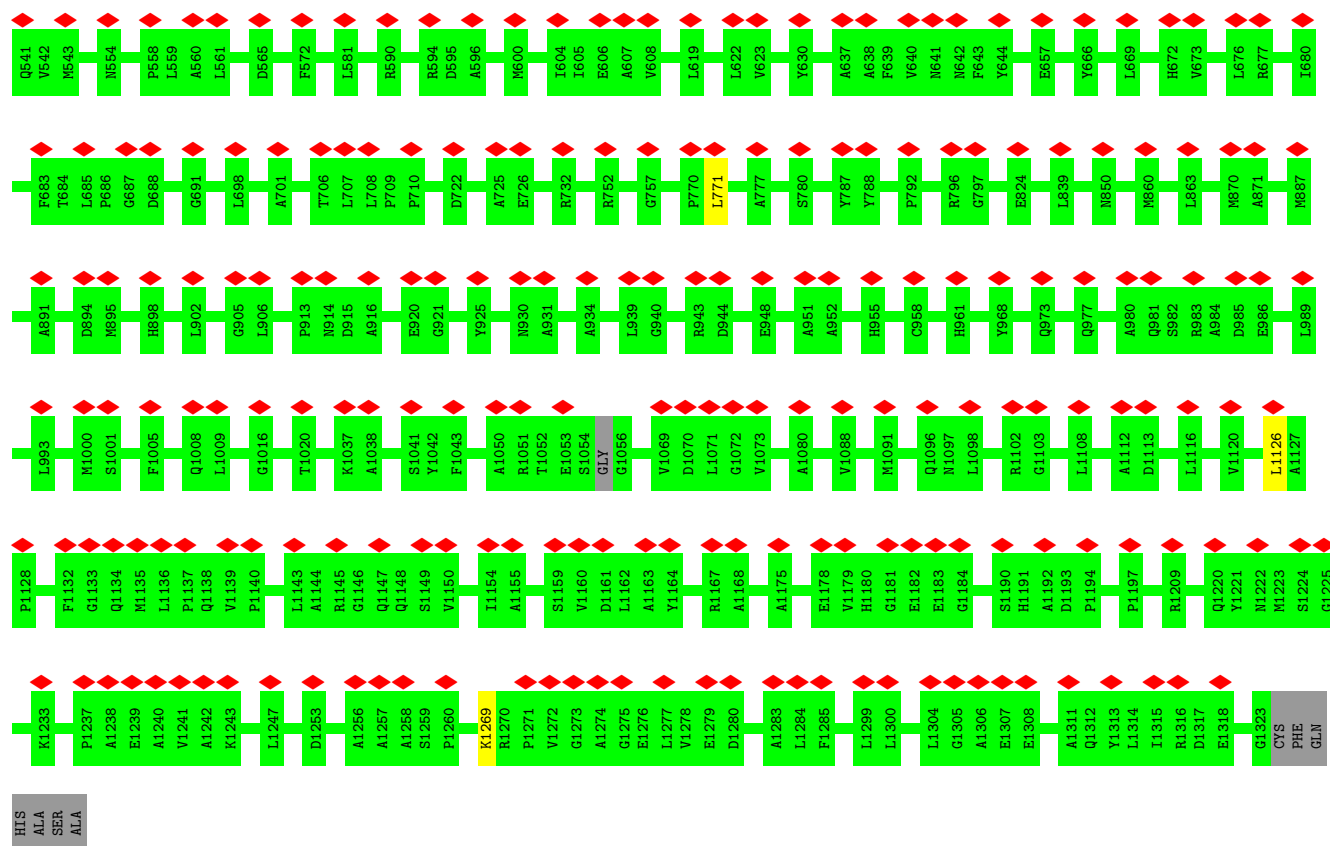
• Molecule 1: Major capsid protein





• Molecule 1: Major capsid protein

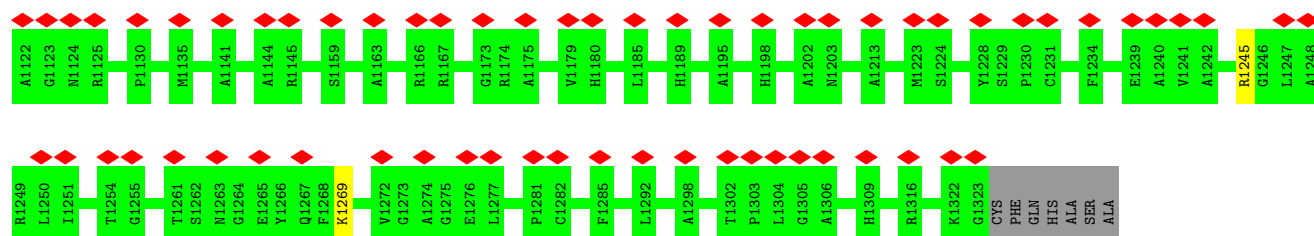




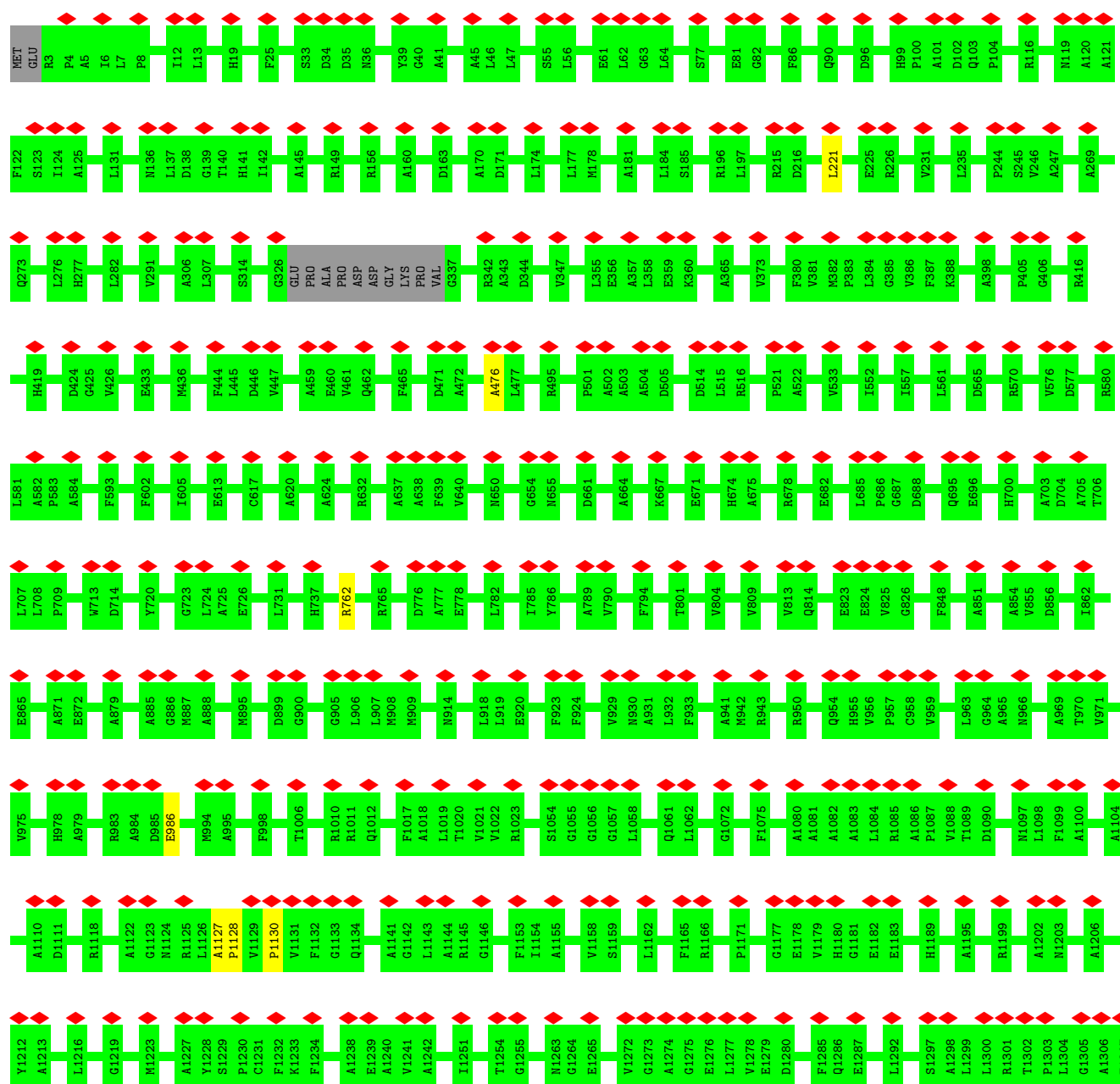
• Molecule 1: Major capsid protein

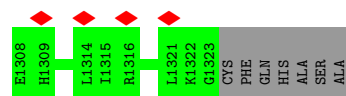




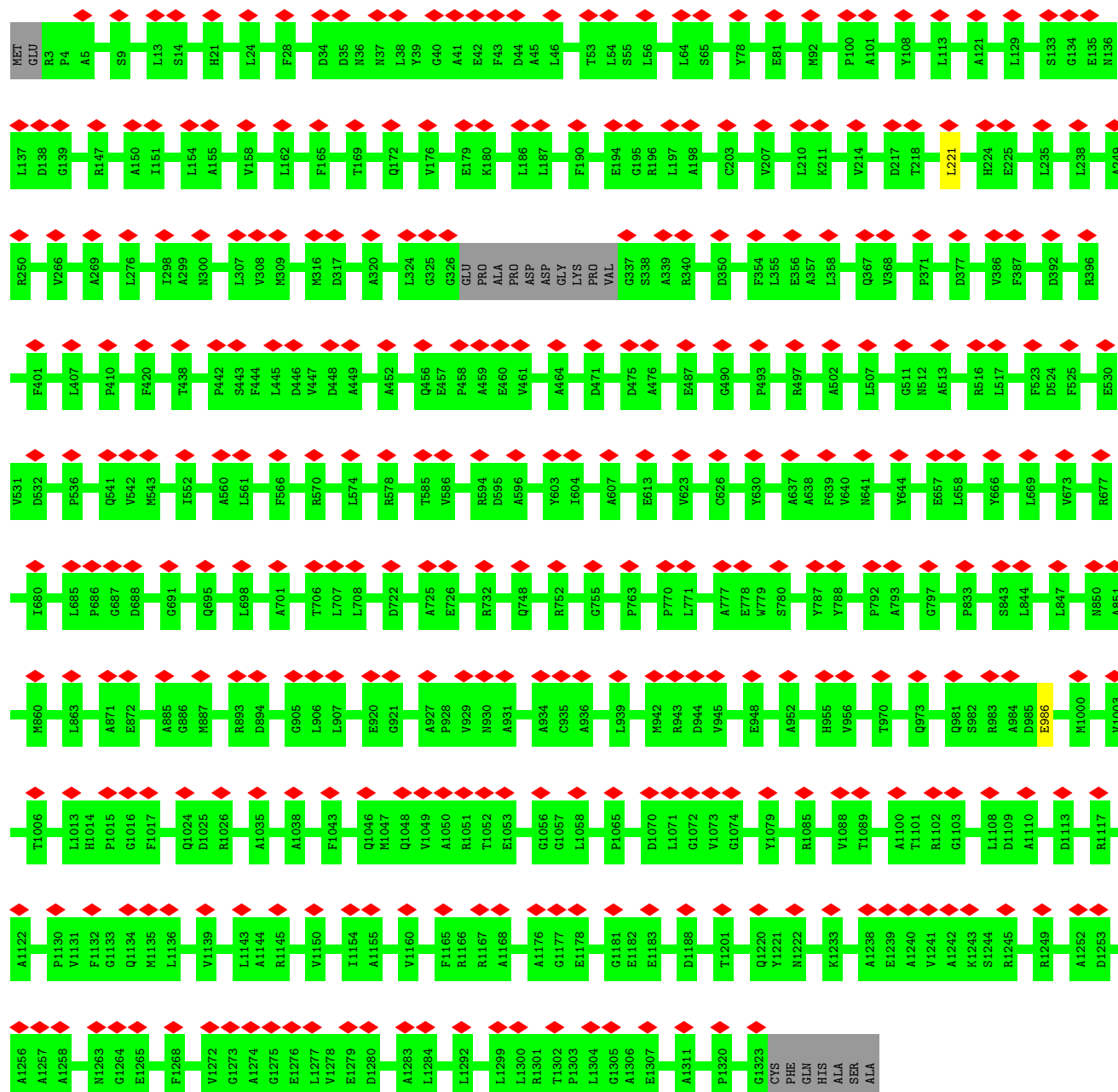


• Molecule 1: Major capsid protein



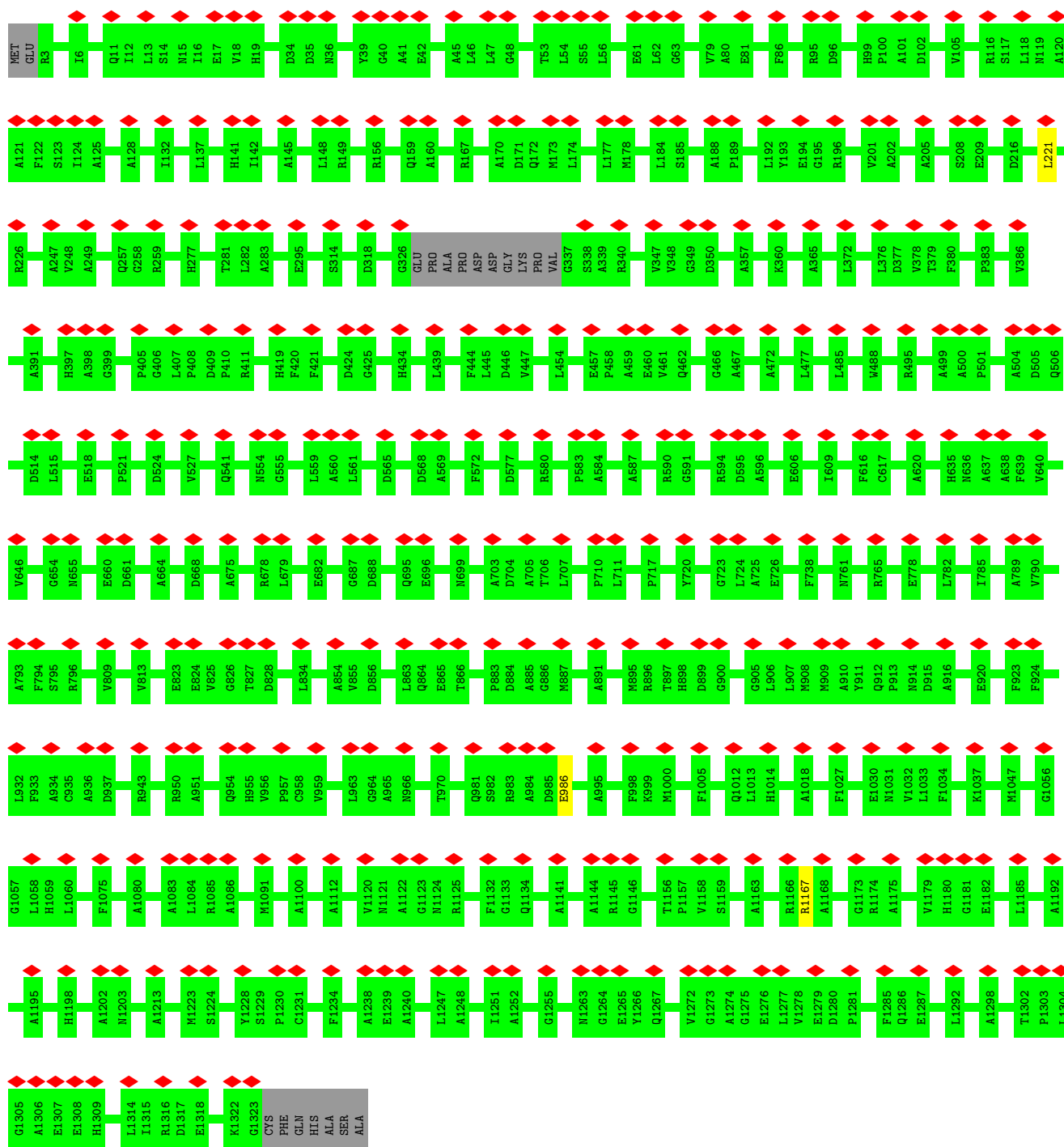


• Molecule 1: Major capsid protein

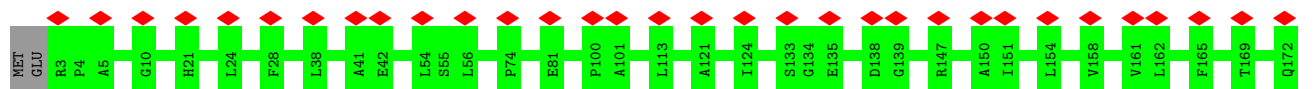


• Molecule 1: Major capsid protein



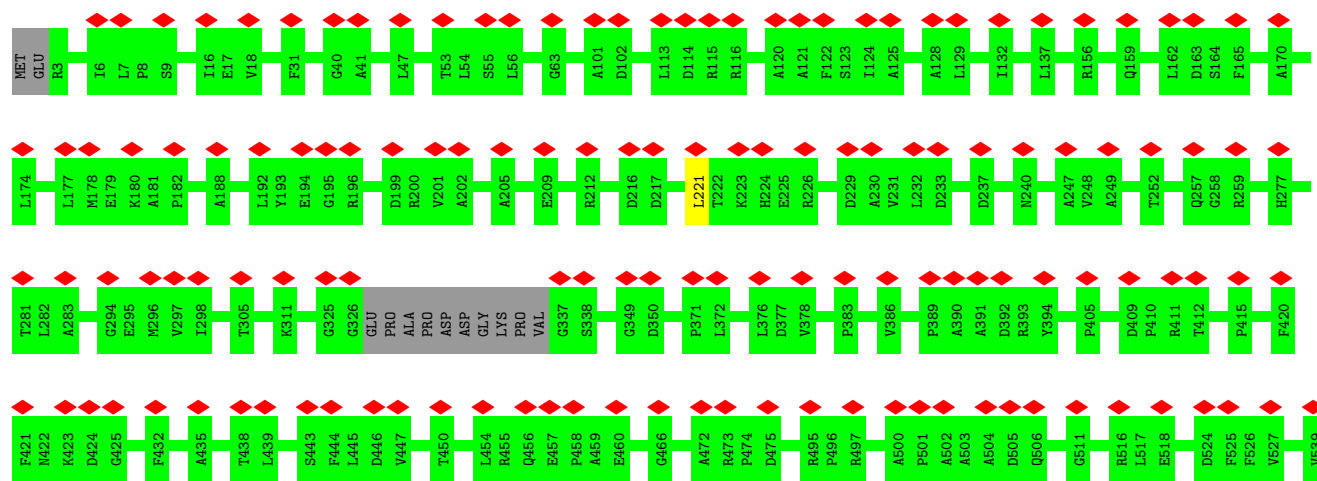


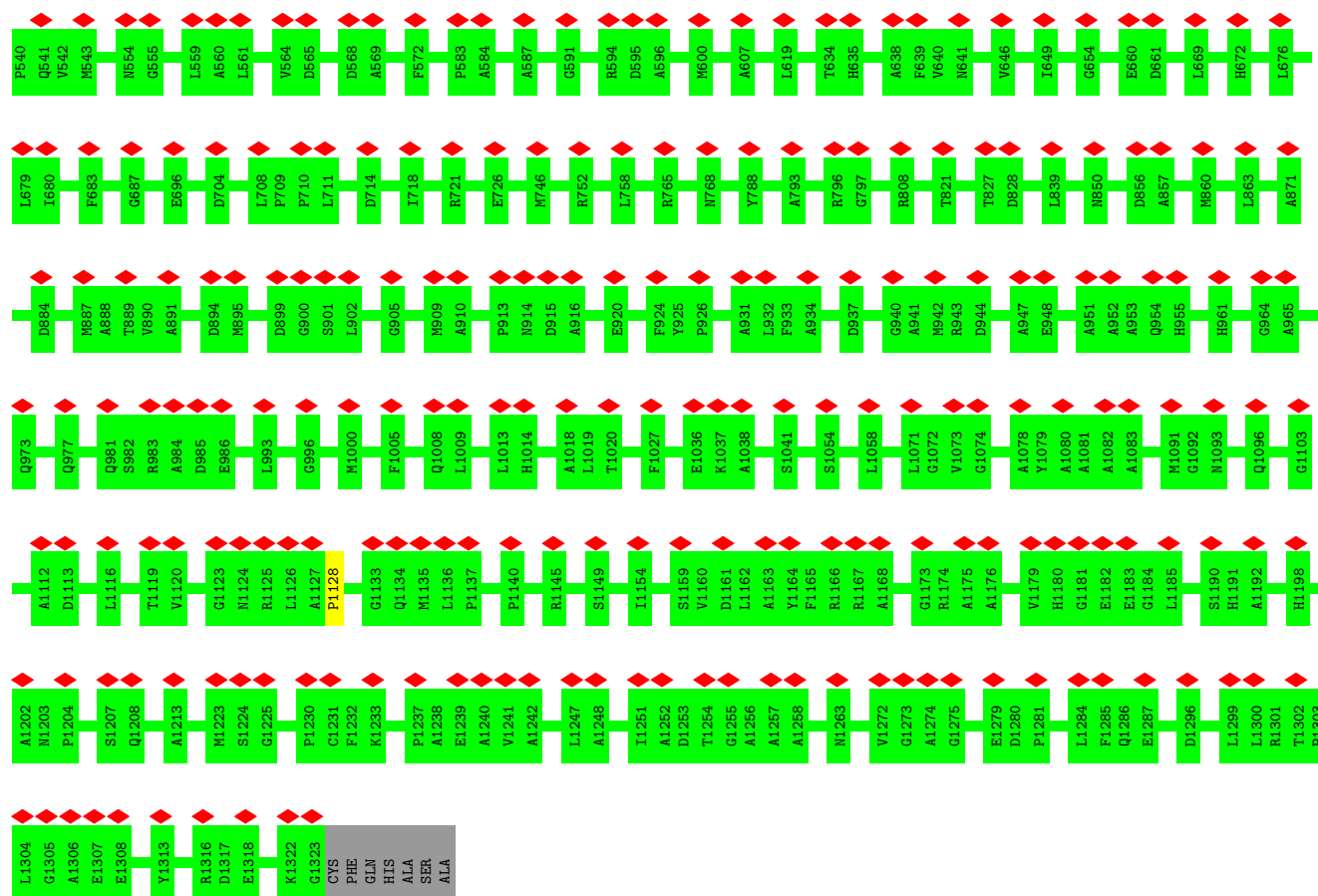
• Molecule 1: Major capsid protein



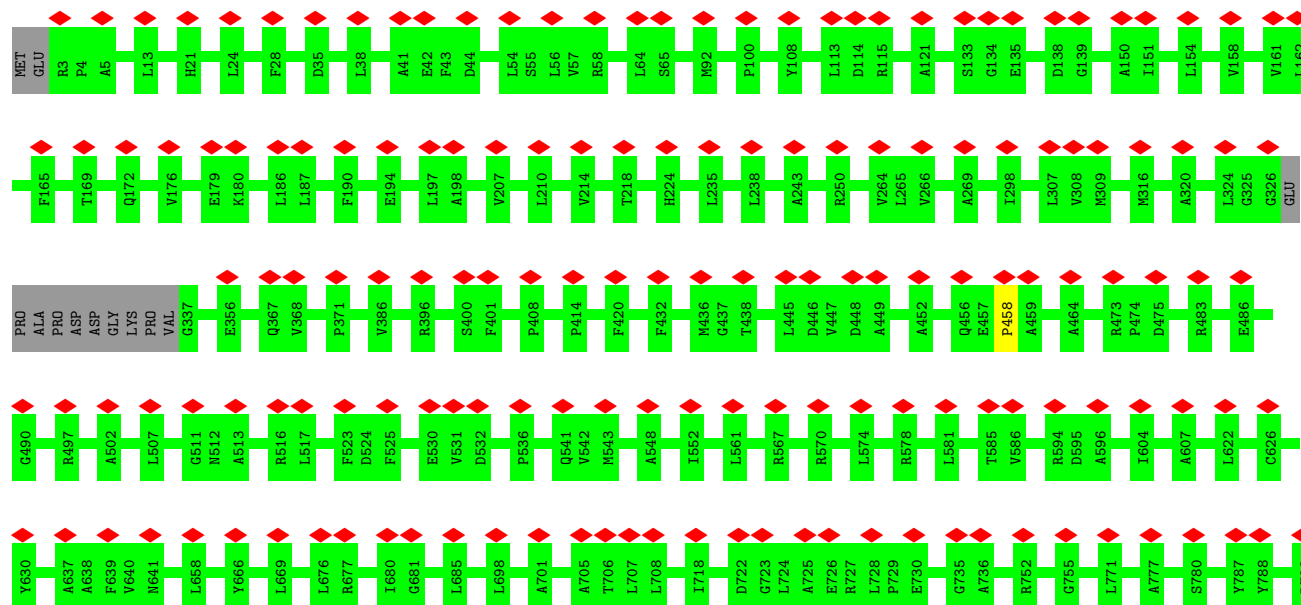


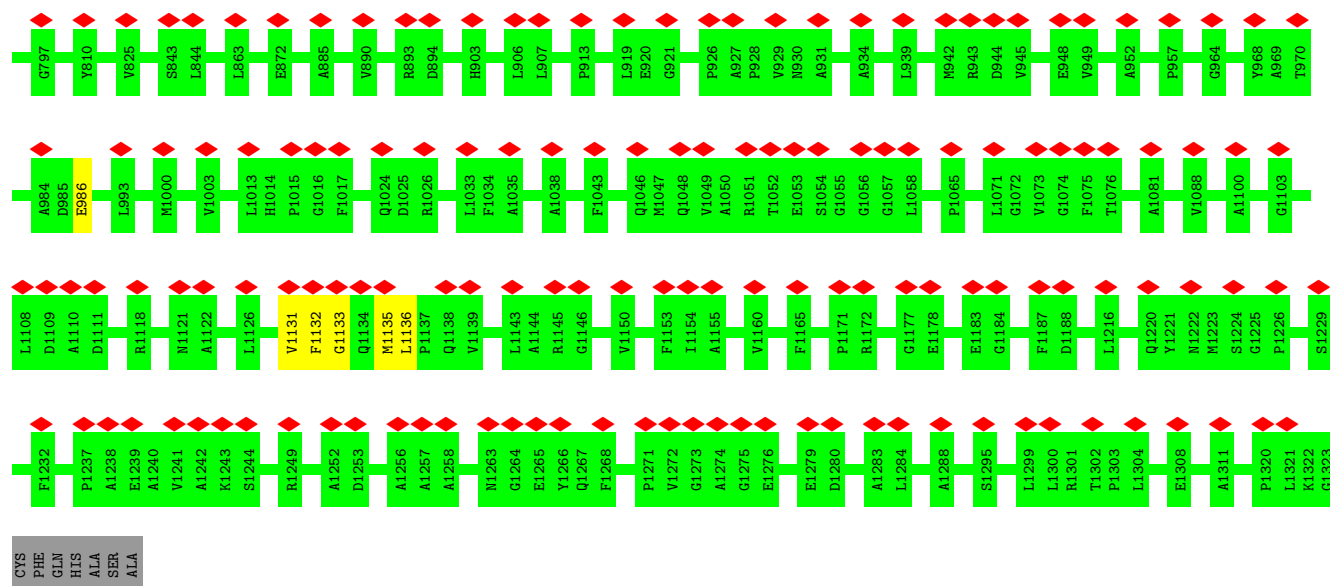
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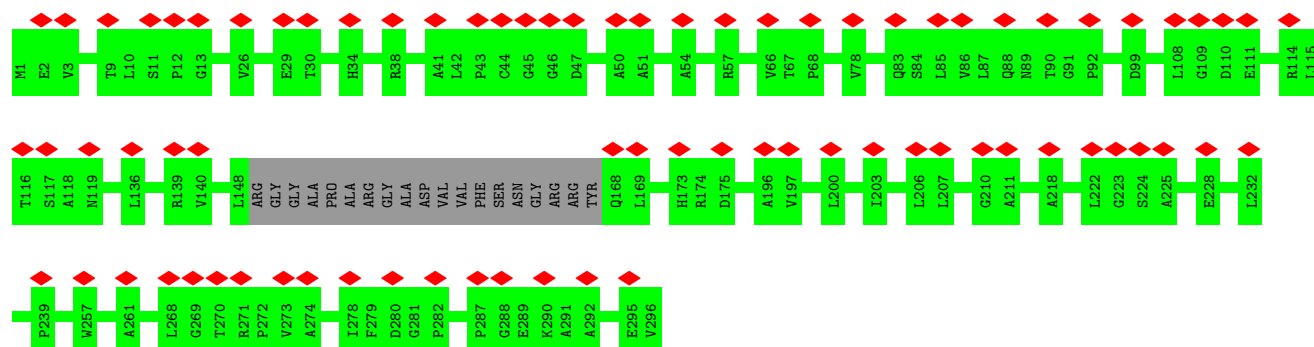


• Molecule 1: Major capsid protein

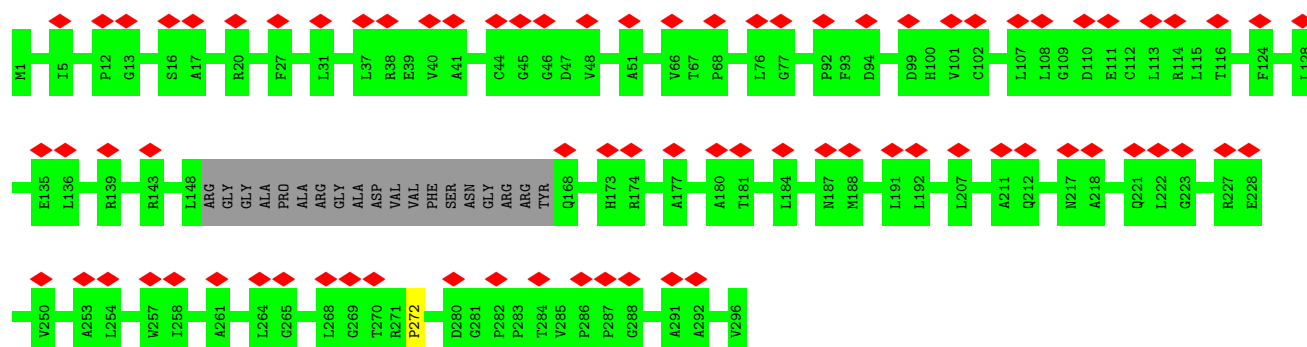




• Molecule 2: Triplex capsid protein 2

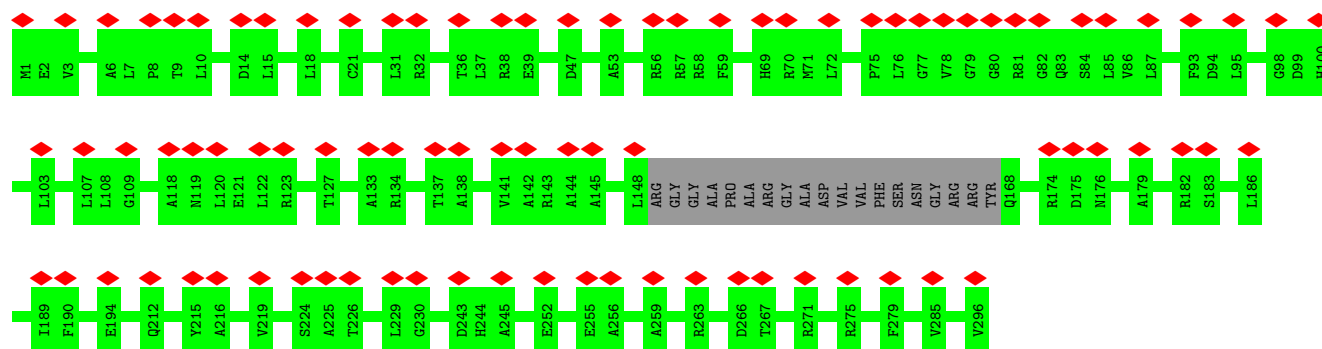


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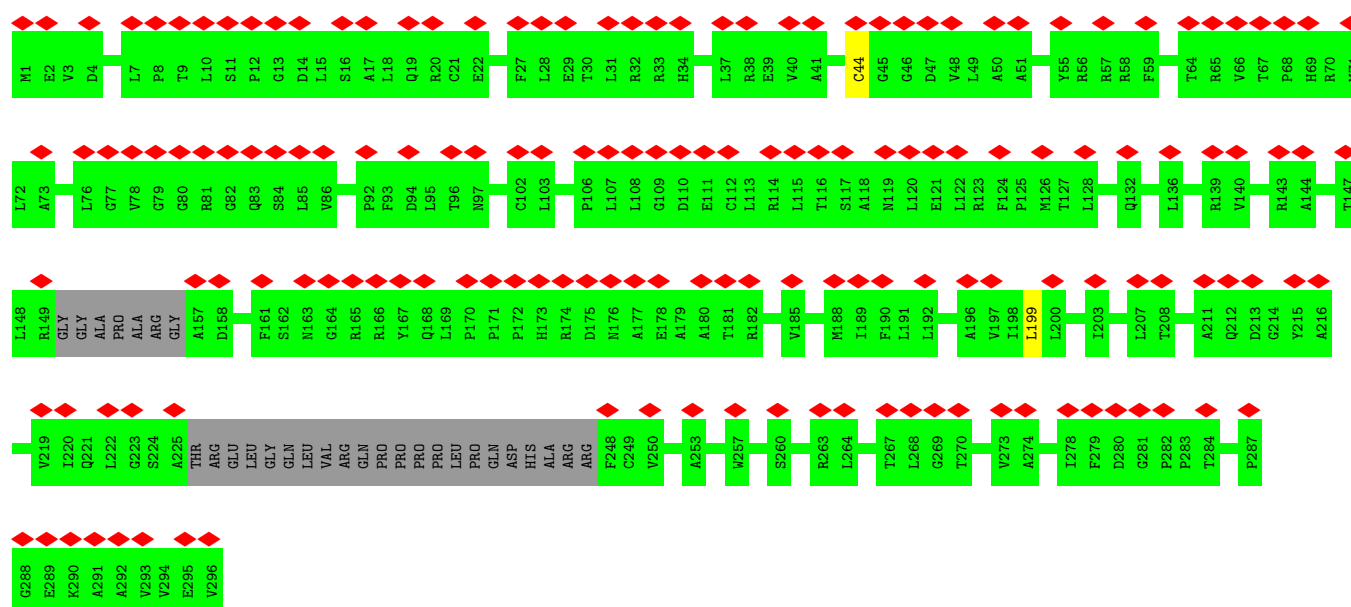
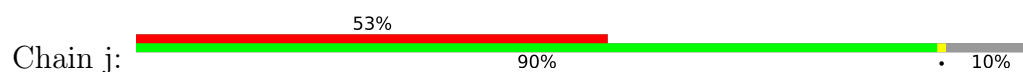


• Molecule 2: Triplex capsid protein 2

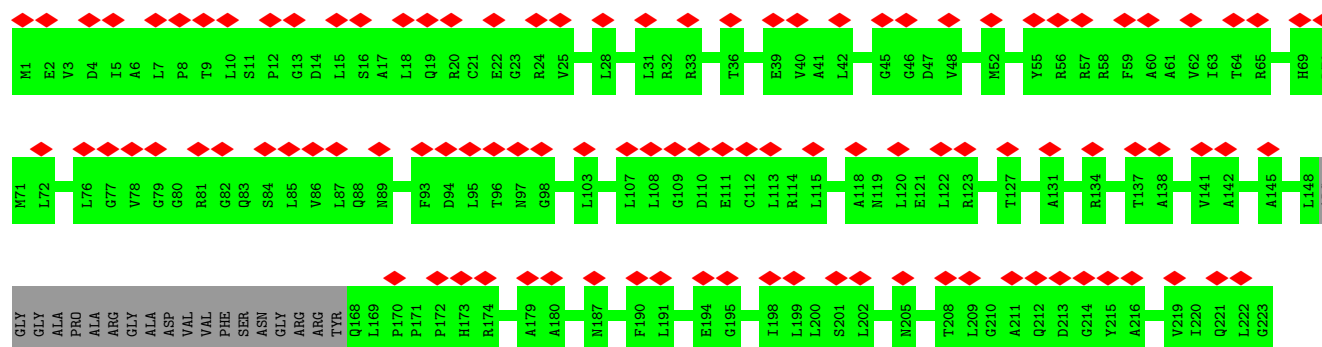


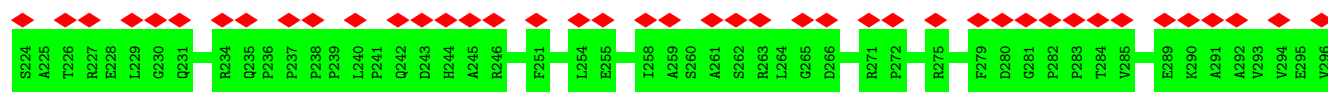


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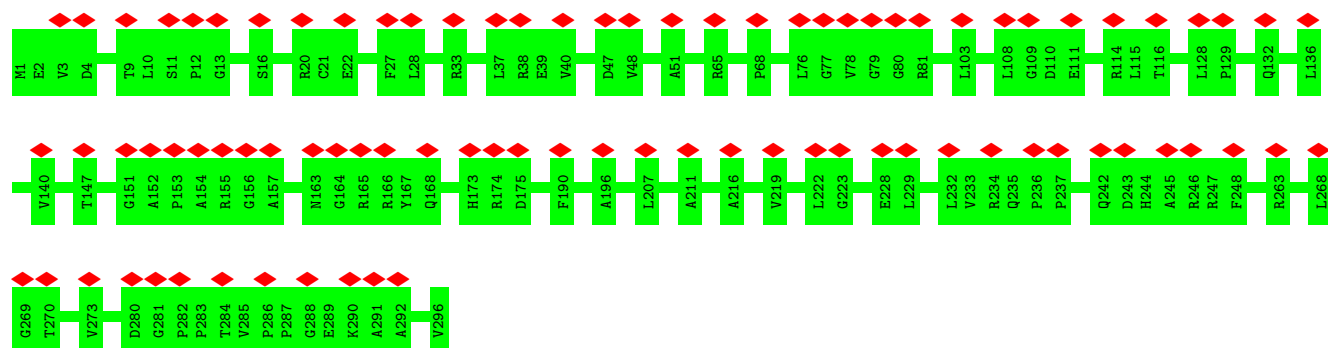


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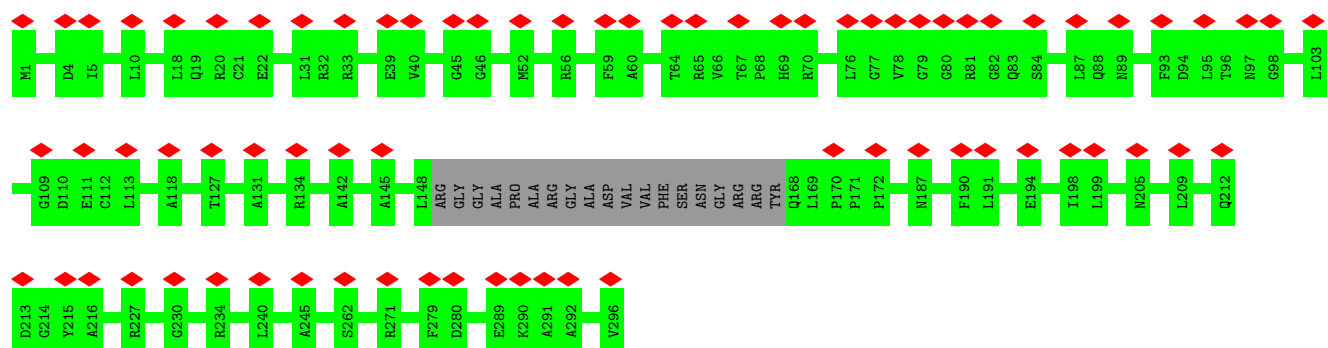




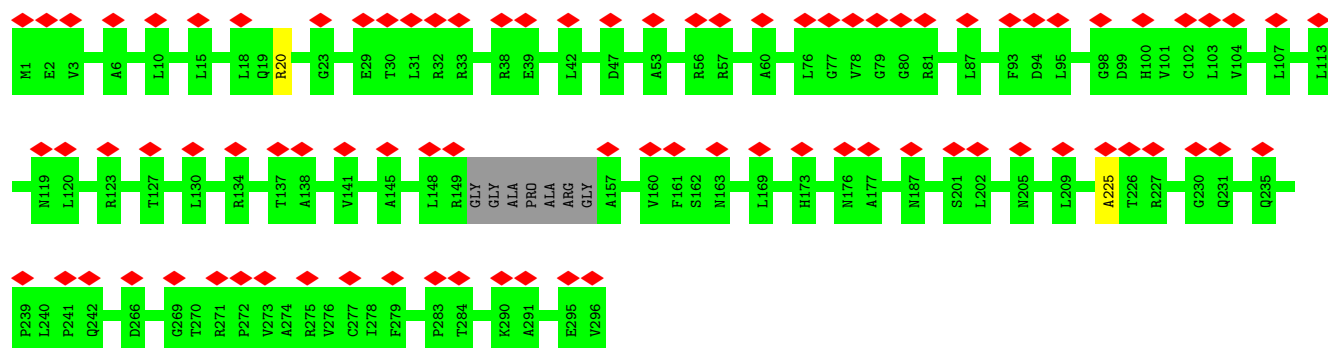
• Molecule 2: Triplex capsid protein 2



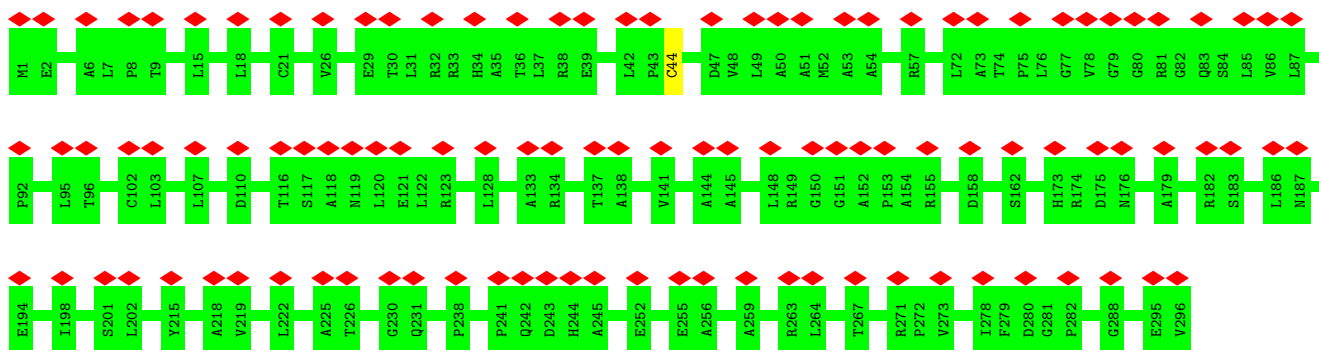
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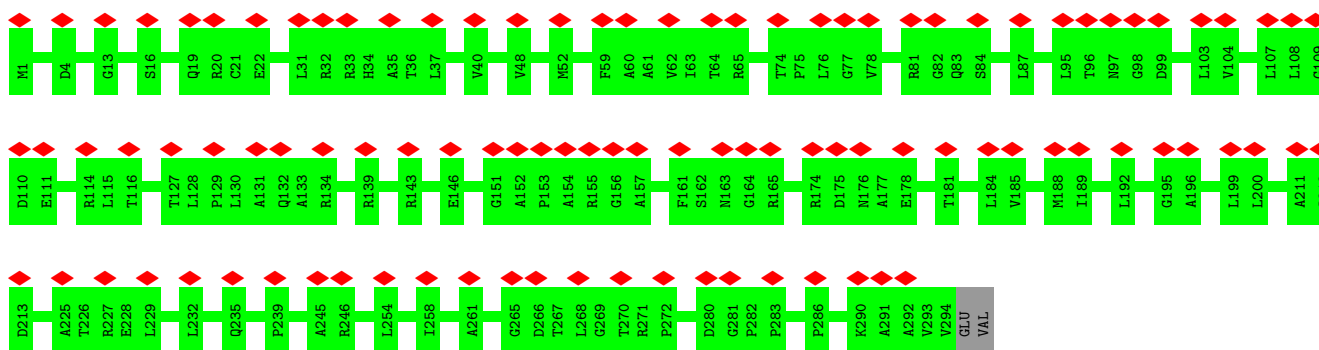
• Molecule 2: Triplex capsid protein 2



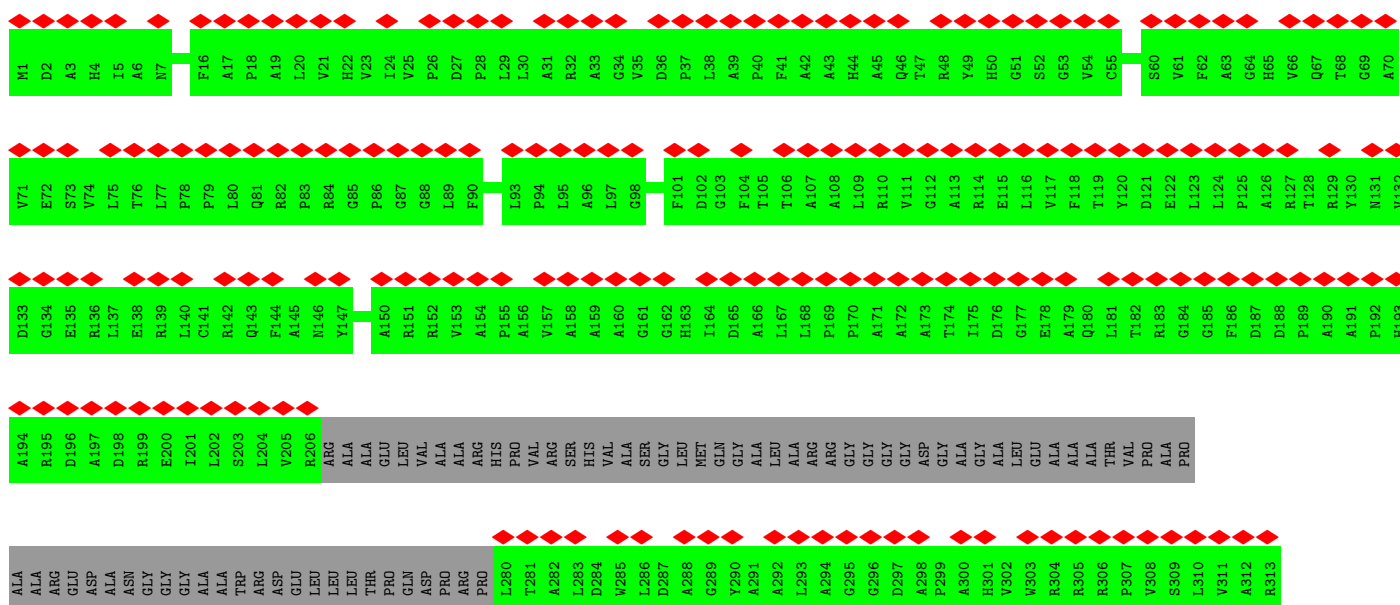
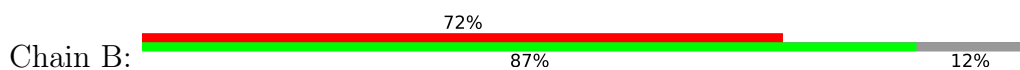
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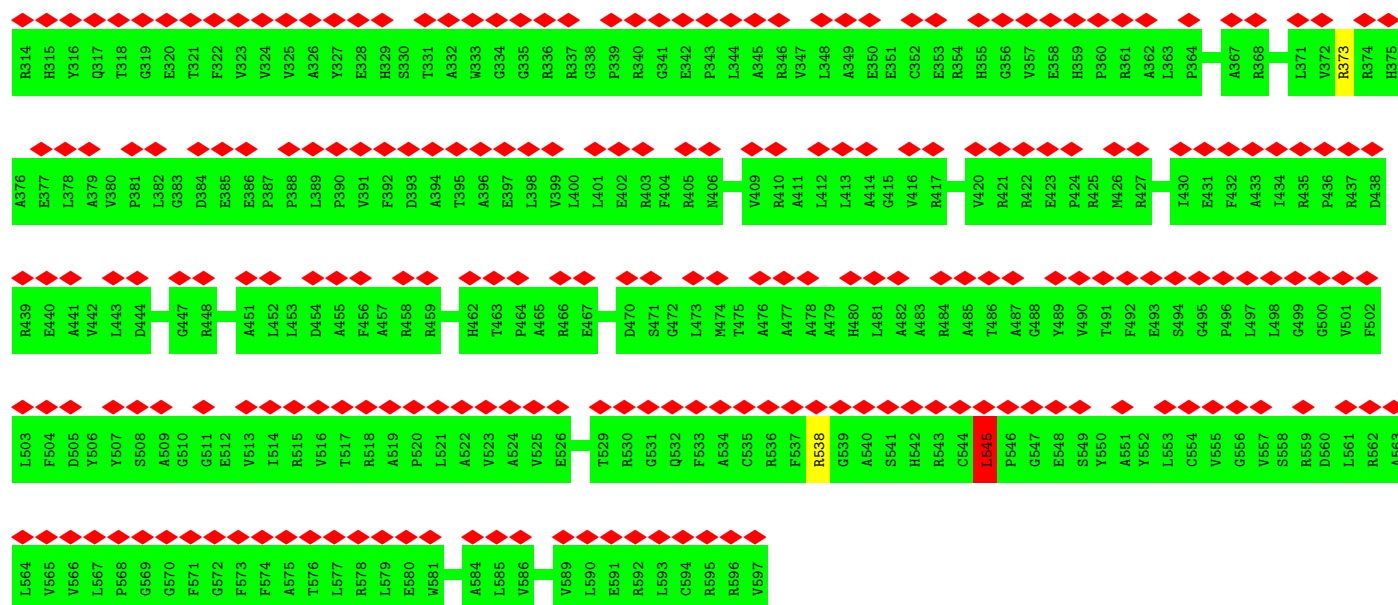


• Molecule 2: Triplex capsid protein 2

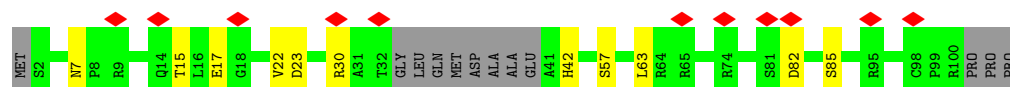
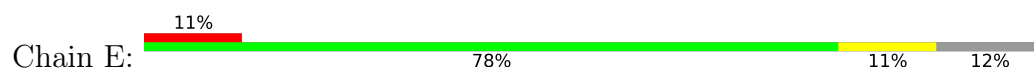


• Molecule 3: Capsid vertex component 1

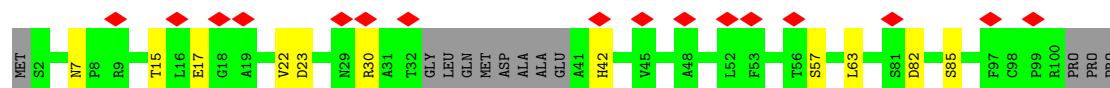
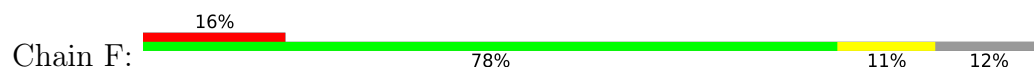




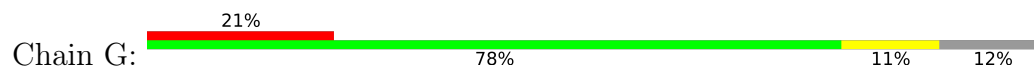
- Molecule 4: Small capsomere-interacting protein



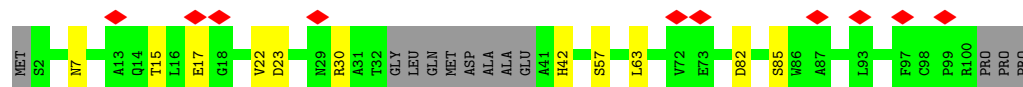
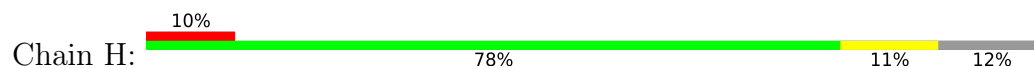
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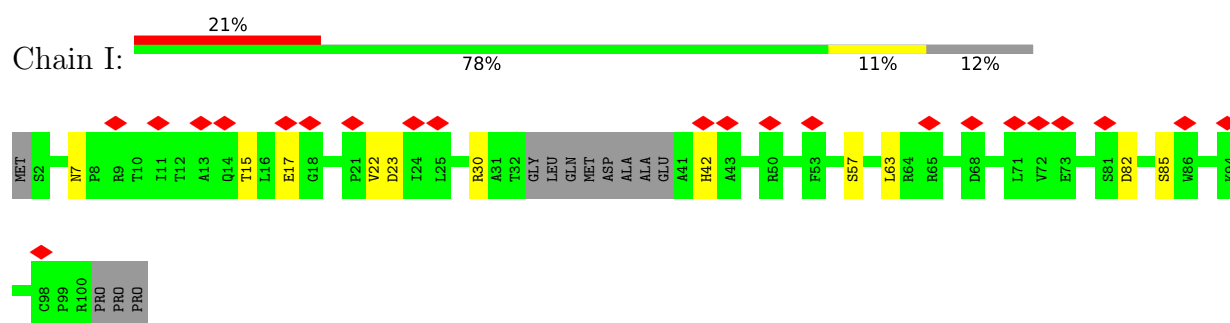
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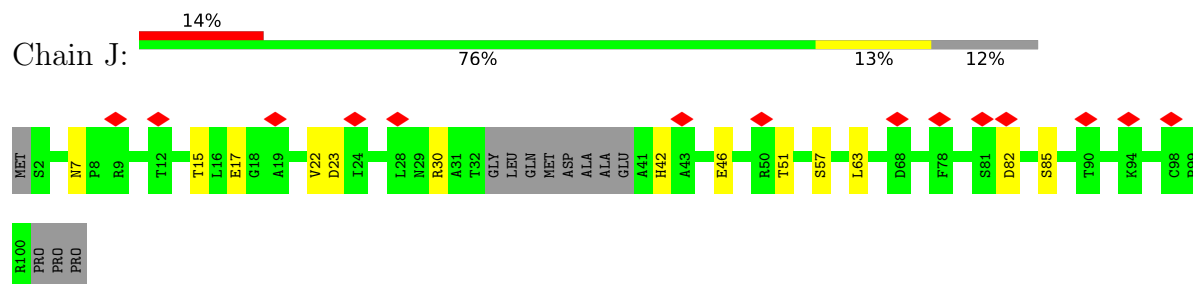
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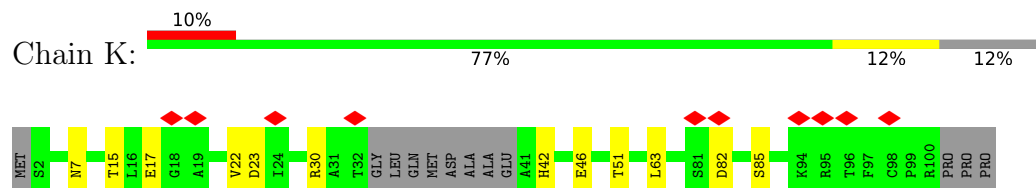
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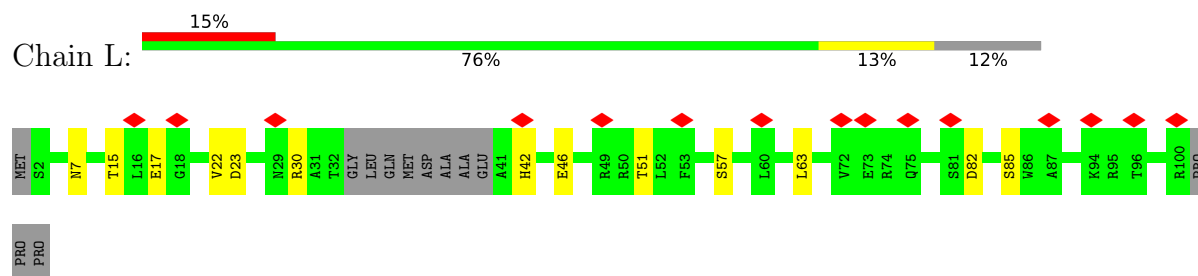
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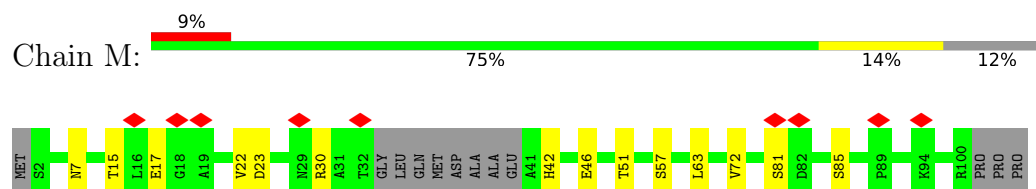
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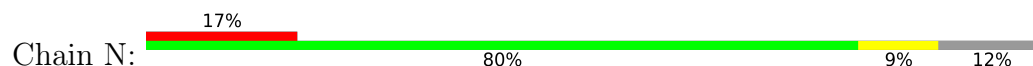
- Molecule 4: Small capsomere-interacting protein

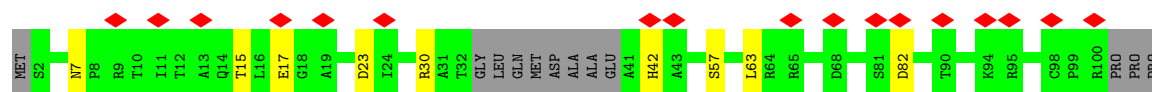


- Molecule 4: Small capsomere-interacting protein

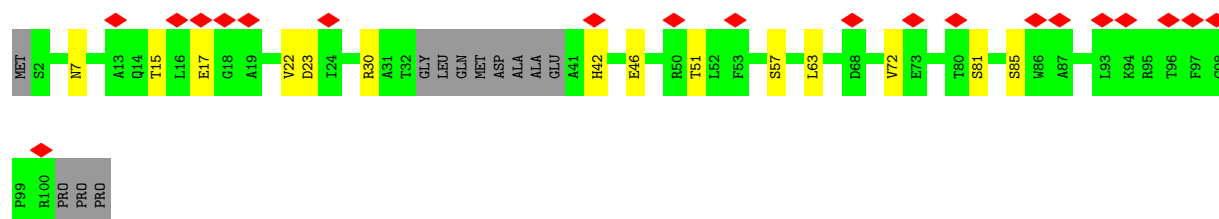
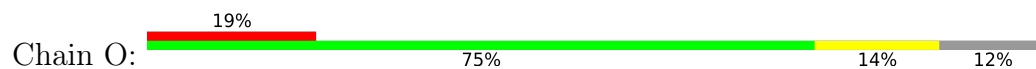


- Molecule 4: Small capsomere-interacting protein

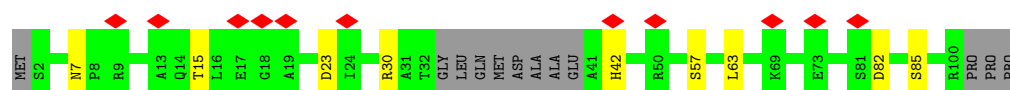
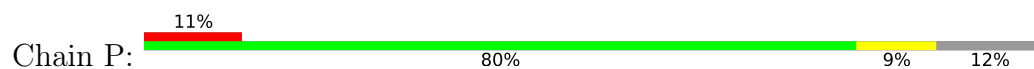




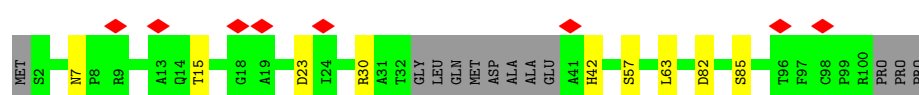
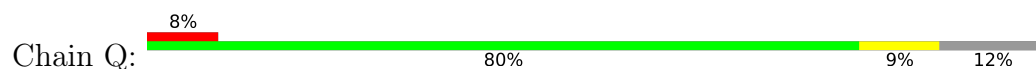
- Molecule 4: Small capsomere-interacting protein



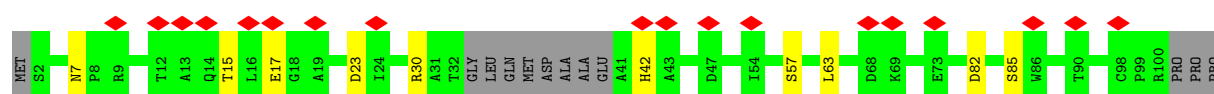
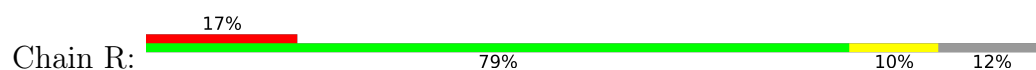
- Molecule 4: Small capsomere-interacting protein



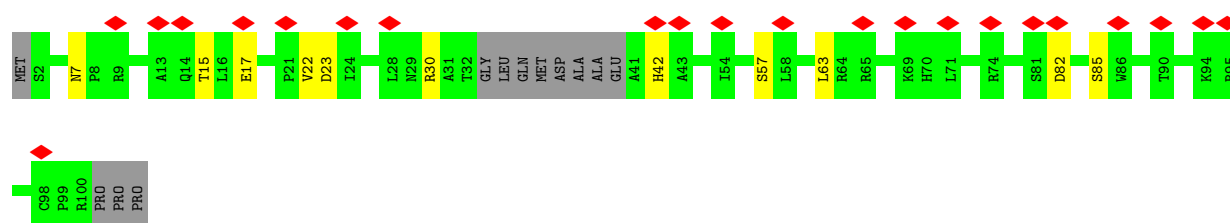
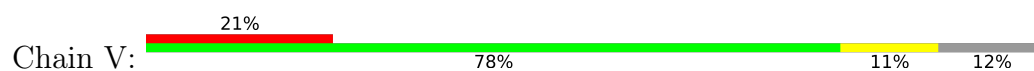
- Molecule 4: Small capsomere-interacting protein




- Molecule 4: Small capsomere-interacting protein

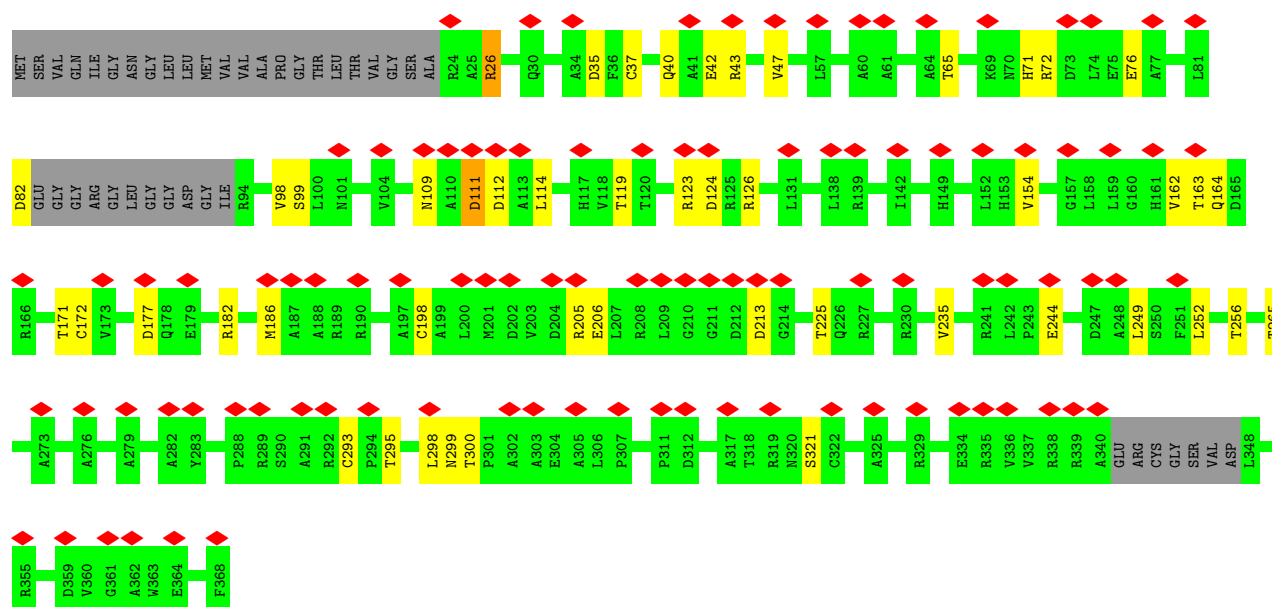


- Molecule 4: Small capsomere-interacting protein




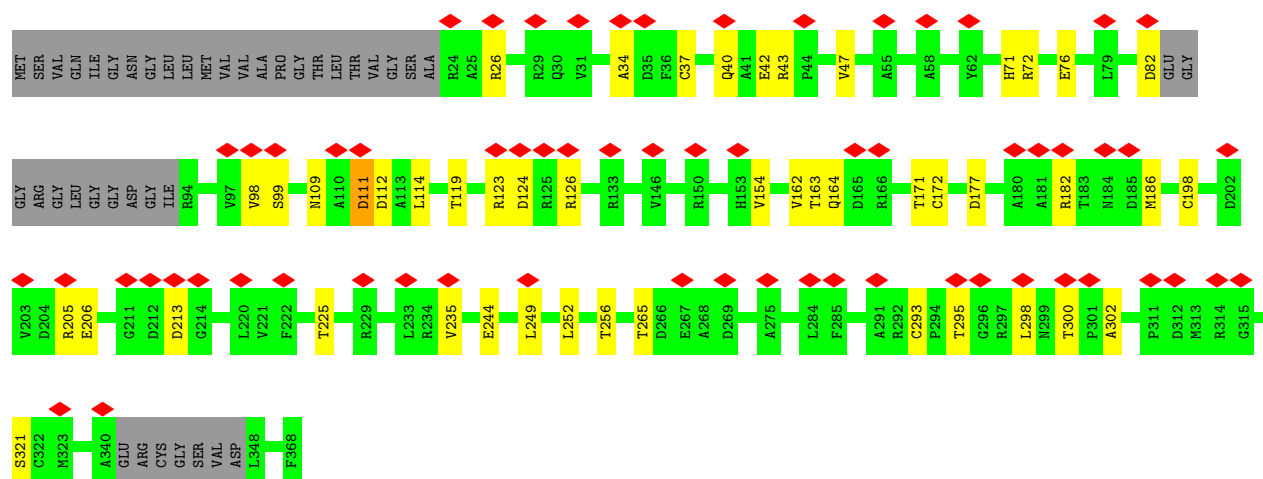
- Molecule 5: Triplex capsid protein 1

Chain T: 




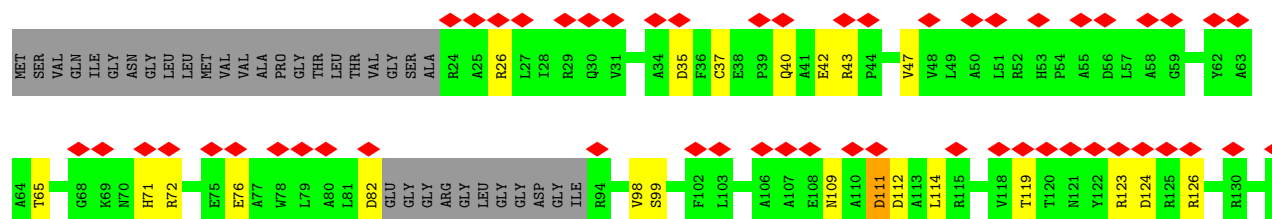
• Molecule 5: Triplex capsid protein 1

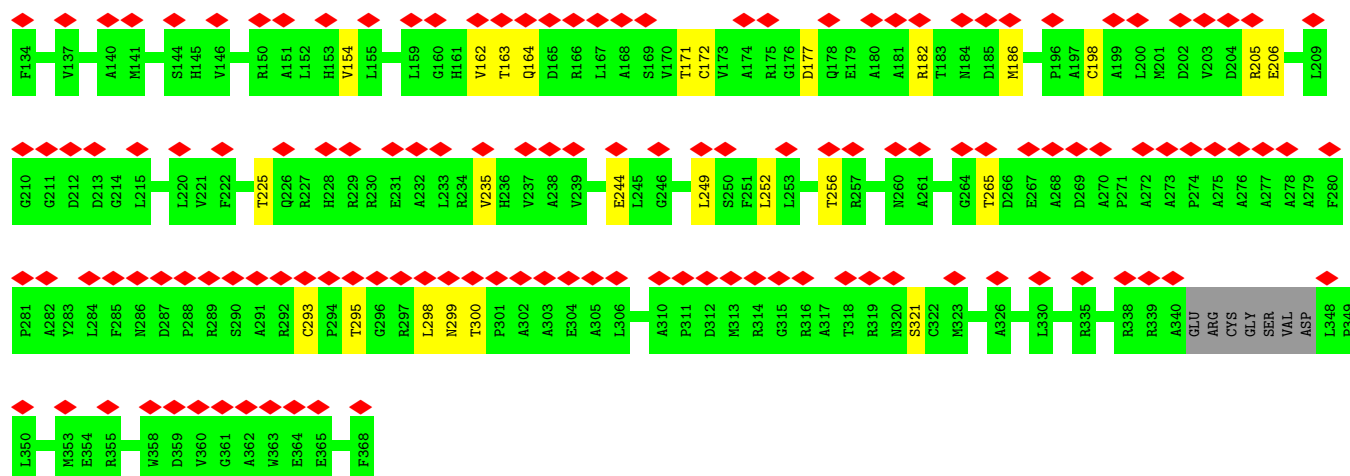
Chain h: 



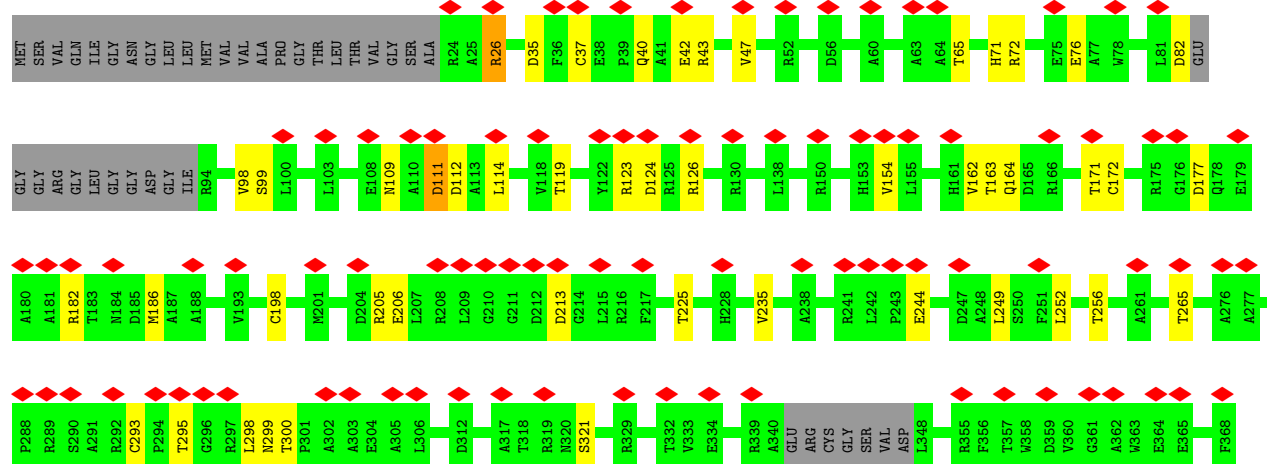
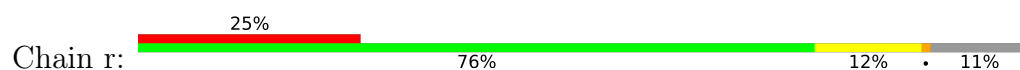
• Molecule 5: Triplex capsid protein 1

Chain i: 

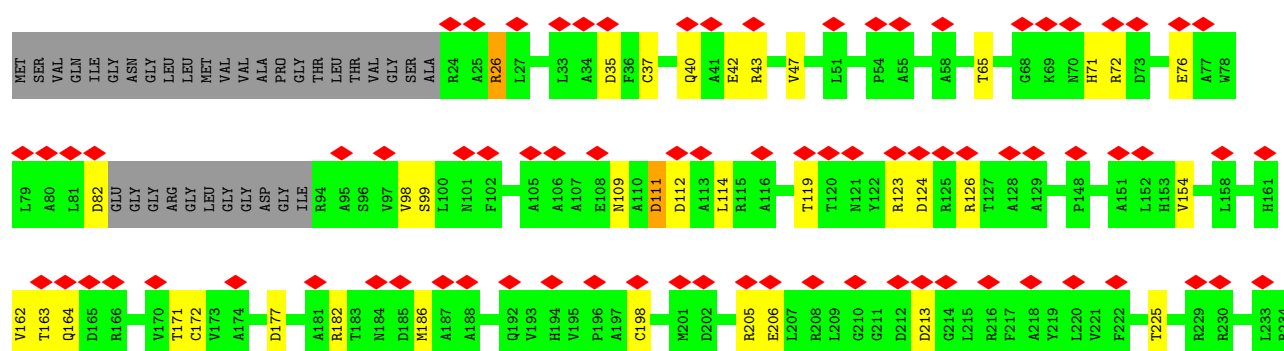
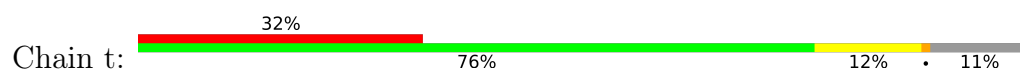


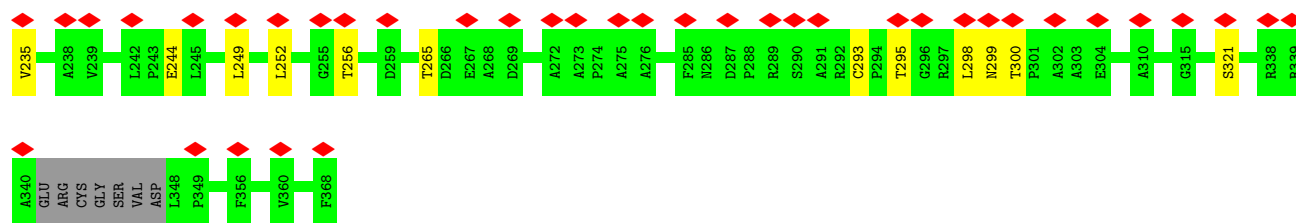


• Molecule 5: Triplex capsid protein 1

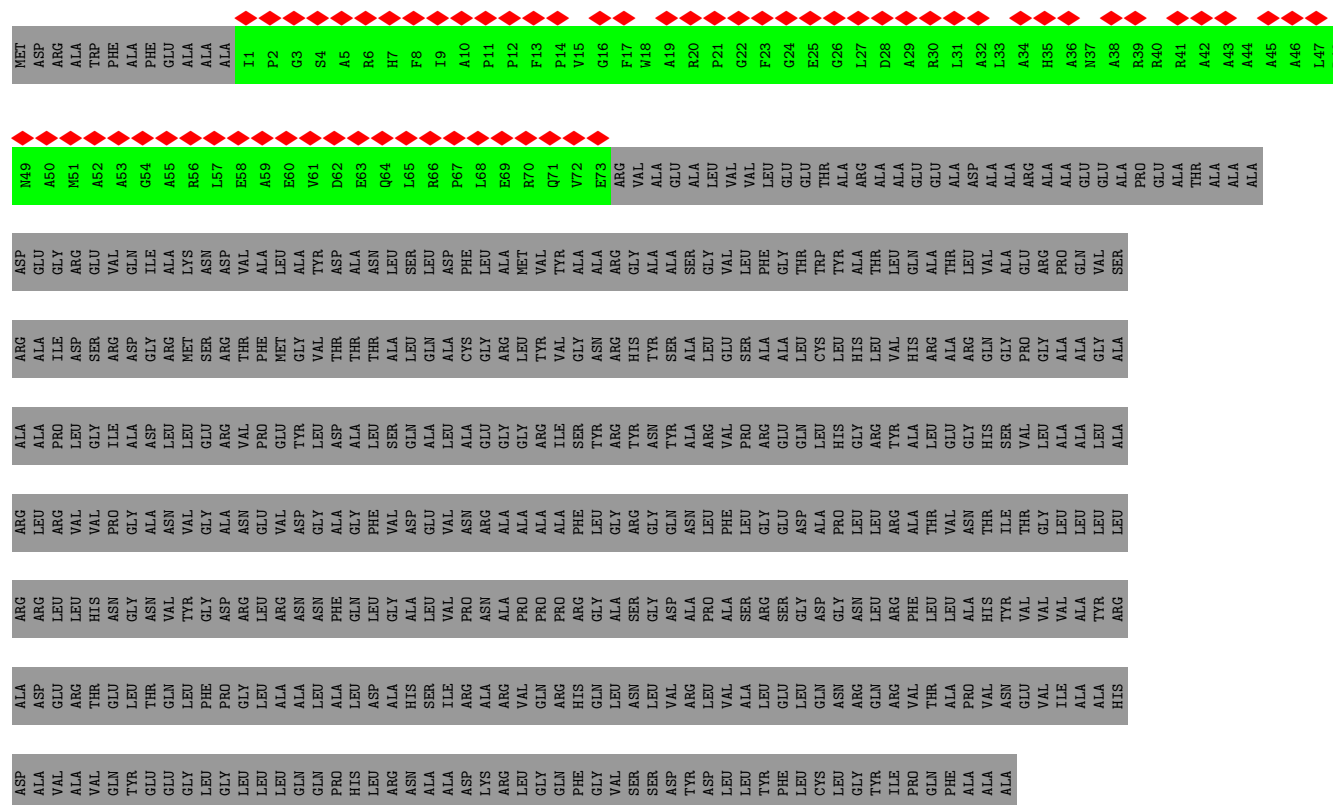


• Molecule 5: Triplex capsid protein 1

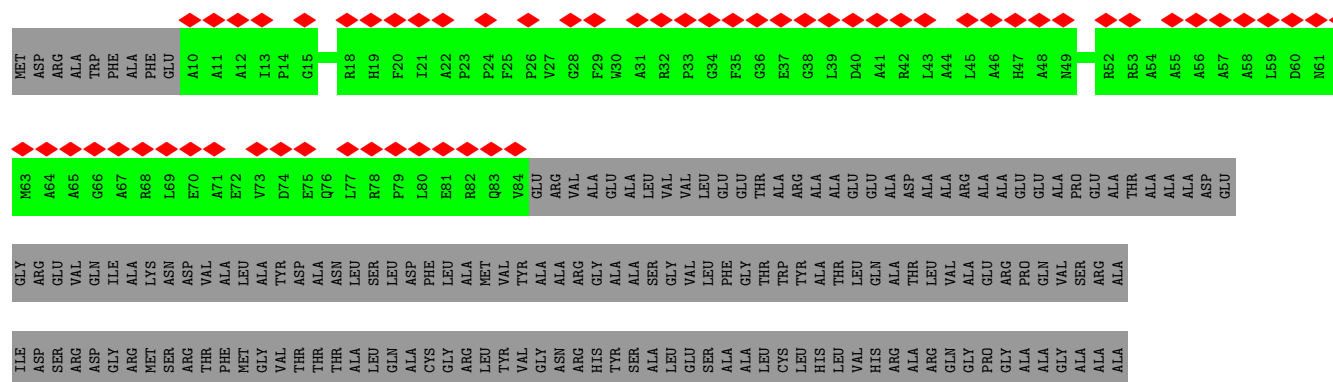




• Molecule 6: DNA packaging tegument protein UL25



• Molecule 6: DNA packaging tegument protein UL25



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14252	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	9.391	Depositor
Minimum map value	-6.027	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.915	Depositor
Recommended contour level	2	Depositor
Map size (Å)	1429.76, 1429.76, 1429.76	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.117, 1.117, 1.117	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	0	0.26	0/10384	0.48	2/14158 (0.0%)
1	A	0.26	0/10366	0.48	1/14132 (0.0%)
1	S	0.26	0/10229	0.48	0/13950
1	U	0.27	0/10384	0.47	1/14158 (0.0%)
1	a	0.26	0/10225	0.46	0/13938
1	e	0.28	0/8938	0.46	0/12175
1	f	0.26	0/10384	0.47	1/14158 (0.0%)
1	g	0.26	0/10379	0.46	2/14150 (0.0%)
1	l	0.26	0/10384	0.47	0/14158
1	m	0.27	0/10384	0.47	1/14158 (0.0%)
1	n	0.28	1/10384 (0.0%)	0.48	3/14158 (0.0%)
1	p	0.26	0/10384	0.47	1/14158 (0.0%)
1	q	0.26	0/10384	0.47	1/14158 (0.0%)
1	u	0.26	0/10384	0.46	1/14158 (0.0%)
1	w	0.26	0/10384	0.47	1/14158 (0.0%)
1	y	0.26	0/10384	0.47	0/14158
2	1	0.31	0/2127	0.50	0/2903
2	2	0.37	1/2127 (0.0%)	0.54	2/2903 (0.1%)
2	3	0.30	0/2127	0.50	0/2903
2	j	0.31	0/2043	0.54	1/2783 (0.0%)
2	k	0.28	0/2127	0.49	0/2903
2	o	0.32	0/2272	0.50	0/3099
2	s	0.33	0/2127	0.49	0/2903
2	v	0.31	0/2230	0.48	0/3041
2	x	0.30	0/2272	0.52	0/3099
2	z	0.29	0/2253	0.50	0/3074
3	B	0.35	0/4120	0.49	0/5609
4	E	0.28	0/736	0.55	0/999
4	F	0.28	0/736	0.58	0/999
4	G	0.29	0/736	0.58	0/999
4	H	0.29	0/736	0.62	0/999
4	I	0.29	0/736	0.63	0/999
4	J	0.29	0/736	0.55	0/999
4	K	0.28	0/736	0.56	0/999

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	L	0.28	0/736	0.59	0/999
4	M	0.28	0/736	0.50	0/999
4	N	0.31	0/736	0.64	1/999 (0.1%)
4	O	0.28	0/736	0.51	0/999
4	P	0.29	0/736	0.64	0/999
4	Q	0.29	0/736	0.64	0/999
4	R	0.29	0/736	0.63	0/999
4	V	0.28	0/736	0.58	0/999
5	T	0.33	0/2591	0.63	2/3521 (0.1%)
5	h	0.33	0/2591	0.65	3/3521 (0.1%)
5	i	0.33	0/2591	0.62	2/3521 (0.1%)
5	r	0.33	0/2591	0.62	2/3521 (0.1%)
5	t	0.33	0/2591	0.62	2/3521 (0.1%)
6	X	0.31	0/565	0.43	0/766
6	c	0.29	0/571	0.41	0/775
7	Y	0.28	0/354	0.48	0/474
7	Z	0.26	0/289	0.47	0/385
All	All	0.28	2/215960 (0.0%)	0.49	30/294293 (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	0	0	1
1	U	0	1
1	e	0	1
1	n	0	2
1	w	0	1
2	v	0	1
3	B	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	n	1130	PRO	N-CD	-11.74	1.31	1.47
2	2	272	PRO	N-CD	10.50	1.62	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	1130	PRO	CA-N-CD	7.38	122.04	111.70
5	T	111	ASP	CB-CG-OD1	-7.36	111.68	118.30
5	i	111	ASP	CB-CG-OD1	-7.31	111.72	118.30
5	h	111	ASP	CB-CG-OD1	-7.27	111.76	118.30
5	t	111	ASP	CB-CG-OD1	-7.26	111.77	118.30
5	r	111	ASP	CB-CG-OD1	-7.21	111.81	118.30
5	i	26	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	n	1130	PRO	N-CA-CB	-7.11	94.77	103.30
5	t	26	ARG	NE-CZ-NH1	7.10	123.85	120.30
5	T	26	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	f	768	ASN	C-N-CA	6.96	139.10	121.70
5	h	26	ARG	NE-CZ-NH1	6.86	123.73	120.30
5	r	26	ARG	NE-CZ-NH1	6.77	123.68	120.30
4	N	17	GLU	CB-CA-C	-5.67	99.06	110.40
1	A	1143	LEU	CA-CB-CG	5.58	128.14	115.30
1	p	221	LEU	CA-CB-CG	5.50	127.96	115.30
1	0	243	ALA	N-CA-CB	5.49	117.79	110.10
1	m	1269	LYS	C-N-CA	-5.45	108.08	121.70
1	w	221	LEU	CA-CB-CG	5.38	127.67	115.30
2	2	272	PRO	CA-N-CD	-5.30	104.08	111.50
1	n	221	LEU	CA-CB-CG	5.27	127.42	115.30
2	2	272	PRO	N-CA-CB	5.27	109.62	103.30
1	0	221	LEU	CA-CB-CG	5.23	127.32	115.30
1	g	1126	LEU	CA-CB-CG	5.21	127.28	115.30
1	g	771	LEU	CA-CB-CG	5.17	127.19	115.30
1	u	221	LEU	CA-CB-CG	5.10	127.02	115.30
5	h	34	ALA	CB-CA-C	-5.09	102.47	110.10
1	U	1126	LEU	CA-CB-CG	5.06	126.94	115.30
1	q	221	LEU	CA-CB-CG	5.03	126.86	115.30
2	j	199	LEU	CA-CB-CG	-5.01	103.77	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	762	ARG	Peptide
3	B	545	LEU	Peptide
1	U	762	ARG	Peptide
1	e	298	ILE	Peptide
1	n	476	ALA	Peptide
1	n	762	ARG	Peptide
2	v	225	ALA	Peptide
1	w	1128	PRO	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	1307/1330 (98%)	1200 (92%)	107 (8%)	0	100	100
1	A	1302/1330 (98%)	1193 (92%)	106 (8%)	3 (0%)	44	78
1	S	1285/1330 (97%)	1174 (91%)	108 (8%)	3 (0%)	44	78
1	U	1307/1330 (98%)	1184 (91%)	122 (9%)	1 (0%)	48	83
1	a	1281/1330 (96%)	1143 (89%)	138 (11%)	0	100	100
1	e	1102/1330 (83%)	993 (90%)	109 (10%)	0	100	100
1	f	1307/1330 (98%)	1182 (90%)	123 (9%)	2 (0%)	44	78
1	g	1304/1330 (98%)	1174 (90%)	130 (10%)	0	100	100
1	l	1307/1330 (98%)	1200 (92%)	106 (8%)	1 (0%)	48	83
1	m	1307/1330 (98%)	1197 (92%)	110 (8%)	0	100	100
1	n	1307/1330 (98%)	1201 (92%)	103 (8%)	3 (0%)	44	78
1	p	1307/1330 (98%)	1199 (92%)	107 (8%)	1 (0%)	48	83
1	q	1307/1330 (98%)	1214 (93%)	92 (7%)	1 (0%)	48	83
1	u	1307/1330 (98%)	1186 (91%)	120 (9%)	1 (0%)	48	83
1	w	1307/1330 (98%)	1189 (91%)	118 (9%)	0	100	100
1	y	1307/1330 (98%)	1190 (91%)	112 (9%)	5 (0%)	30	68
2	1	273/296 (92%)	252 (92%)	21 (8%)	0	100	100
2	2	273/296 (92%)	251 (92%)	22 (8%)	0	100	100
2	3	273/296 (92%)	250 (92%)	23 (8%)	0	100	100
2	j	261/296 (88%)	236 (90%)	25 (10%)	0	100	100
2	k	273/296 (92%)	252 (92%)	21 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	o	294/296 (99%)	264 (90%)	30 (10%)	0	100	100
2	s	273/296 (92%)	248 (91%)	25 (9%)	0	100	100
2	v	285/296 (96%)	256 (90%)	29 (10%)	0	100	100
2	x	294/296 (99%)	257 (87%)	37 (13%)	0	100	100
2	z	292/296 (99%)	260 (89%)	32 (11%)	0	100	100
3	B	520/597 (87%)	459 (88%)	60 (12%)	1 (0%)	44	78
4	E	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	F	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	G	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	H	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	I	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	J	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	K	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	L	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	M	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	N	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	O	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	P	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	Q	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	R	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	V	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
5	T	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
5	h	321/368 (87%)	294 (92%)	26 (8%)	1 (0%)	37	72
5	i	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
5	r	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
5	t	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
6	X	71/534 (13%)	67 (94%)	4 (6%)	0	100	100
6	c	73/534 (14%)	67 (92%)	6 (8%)	0	100	100
7	Y	43/62 (69%)	42 (98%)	1 (2%)	0	100	100
7	Z	33/62 (53%)	32 (97%)	1 (3%)	0	100	100
All	All	27092/29414 (92%)	24684 (91%)	2385 (9%)	23 (0%)	50	83

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	h	302	ALA
1	U	986	GLU
1	n	1127	ALA
1	p	986	GLU
1	y	986	GLU
1	A	986	GLU
1	S	1227	ALA
1	f	986	GLU
1	l	986	GLU
1	n	986	GLU
1	n	1128	PRO
1	q	986	GLU
1	u	1126	LEU
3	B	545	LEU
1	y	1133	GLY
1	y	1135	MET
1	y	1131	VAL
1	A	1265	GLU
1	S	1226	PRO
1	S	735	GLY
1	f	1128	PRO
1	A	1137	PRO
1	y	458	PRO

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	0	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	A	1056/1072 (98%)	1056 (100%)	0	100	100
1	S	1042/1072 (97%)	1042 (100%)	0	100	100
1	U	1057/1072 (99%)	1057 (100%)	0	100	100
1	a	1040/1072 (97%)	1040 (100%)	0	100	100
1	e	909/1072 (85%)	909 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	g	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	l	1057/1072 (99%)	1057 (100%)	0	100	100
1	m	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	n	1057/1072 (99%)	1057 (100%)	0	100	100
1	p	1057/1072 (99%)	1057 (100%)	0	100	100
1	q	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	u	1057/1072 (99%)	1057 (100%)	0	100	100
1	w	1057/1072 (99%)	1057 (100%)	0	100	100
1	y	1057/1072 (99%)	1055 (100%)	2 (0%)	92	93
2	1	223/235 (95%)	223 (100%)	0	100	100
2	2	223/235 (95%)	223 (100%)	0	100	100
2	3	223/235 (95%)	223 (100%)	0	100	100
2	j	213/235 (91%)	212 (100%)	1 (0%)	86	89
2	k	223/235 (95%)	223 (100%)	0	100	100
2	o	235/235 (100%)	235 (100%)	0	100	100
2	s	223/235 (95%)	223 (100%)	0	100	100
2	v	233/235 (99%)	232 (100%)	1 (0%)	89	90
2	x	235/235 (100%)	234 (100%)	1 (0%)	89	90
2	z	232/235 (99%)	232 (100%)	0	100	100
3	B	396/440 (90%)	393 (99%)	3 (1%)	79	84
4	E	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	F	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	G	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	H	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	I	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	J	78/87 (90%)	65 (83%)	13 (17%)	2	10
4	K	78/87 (90%)	66 (85%)	12 (15%)	2	12
4	L	78/87 (90%)	65 (83%)	13 (17%)	2	10
4	M	78/87 (90%)	64 (82%)	14 (18%)	1	9
4	N	78/87 (90%)	70 (90%)	8 (10%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	78/87 (90%)	64 (82%)	14 (18%)	1	9
4	P	78/87 (90%)	69 (88%)	9 (12%)	4	18
4	Q	78/87 (90%)	69 (88%)	9 (12%)	4	18
4	R	78/87 (90%)	68 (87%)	10 (13%)	3	15
4	V	78/87 (90%)	67 (86%)	11 (14%)	3	14
5	T	251/279 (90%)	203 (81%)	48 (19%)	1	7
5	h	251/279 (90%)	207 (82%)	44 (18%)	1	9
5	i	251/279 (90%)	205 (82%)	46 (18%)	1	8
5	r	251/279 (90%)	203 (81%)	48 (19%)	1	7
5	t	251/279 (90%)	203 (81%)	48 (19%)	1	7
6	X	49/387 (13%)	49 (100%)	0	100	100
6	c	48/387 (12%)	48 (100%)	0	100	100
7	Y	36/51 (71%)	36 (100%)	0	100	100
7	Z	30/51 (59%)	30 (100%)	0	100	100
All	All	21978/23518 (94%)	21563 (98%)	415 (2%)	52	69

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	226	ARG
3	B	373	ARG
3	B	538	ARG
3	B	545	LEU
4	E	7	ASN
4	E	15	THR
4	E	17	GLU
4	E	22	VAL
4	E	23	ASP
4	E	30	ARG
4	E	42	HIS
4	E	57	SER
4	E	63	LEU
4	E	82	ASP
4	E	85	SER
4	F	7	ASN
4	F	15	THR
4	F	17	GLU

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Mol	Chain	Res	Type
4	F	22	VAL
4	F	23	ASP
4	F	30	ARG
4	F	42	HIS
4	F	57	SER
4	F	63	LEU
4	F	82	ASP
4	F	85	SER
4	G	7	ASN
4	G	15	THR
4	G	17	GLU
4	G	22	VAL
4	G	23	ASP
4	G	30	ARG
4	G	42	HIS
4	G	57	SER
4	G	63	LEU
4	G	82	ASP
4	G	85	SER
4	H	7	ASN
4	H	15	THR
4	H	17	GLU
4	H	22	VAL
4	H	23	ASP
4	H	30	ARG
4	H	42	HIS
4	H	57	SER
4	H	63	LEU
4	H	82	ASP
4	H	85	SER
4	I	7	ASN
4	I	15	THR
4	I	17	GLU
4	I	22	VAL
4	I	23	ASP
4	I	30	ARG
4	I	42	HIS
4	I	57	SER
4	I	63	LEU
4	I	82	ASP
4	I	85	SER
4	J	7	ASN

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Mol	Chain	Res	Type
4	J	15	THR
4	J	17	GLU
4	J	22	VAL
4	J	23	ASP
4	J	30	ARG
4	J	42	HIS
4	J	46	GLU
4	J	51	THR
4	J	57	SER
4	J	63	LEU
4	J	82	ASP
4	J	85	SER
4	K	7	ASN
4	K	15	THR
4	K	17	GLU
4	K	22	VAL
4	K	23	ASP
4	K	30	ARG
4	K	42	HIS
4	K	46	GLU
4	K	51	THR
4	K	63	LEU
4	K	82	ASP
4	K	85	SER
4	L	7	ASN
4	L	15	THR
4	L	17	GLU
4	L	22	VAL
4	L	23	ASP
4	L	30	ARG
4	L	42	HIS
4	L	46	GLU
4	L	51	THR
4	L	57	SER
4	L	63	LEU
4	L	82	ASP
4	L	85	SER
4	M	7	ASN
4	M	15	THR
4	M	17	GLU
4	M	22	VAL
4	M	23	ASP

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Mol	Chain	Res	Type
4	M	30	ARG
4	M	42	HIS
4	M	46	GLU
4	M	51	THR
4	M	57	SER
4	M	63	LEU
4	M	72	VAL
4	M	81	SER
4	M	85	SER
4	N	7	ASN
4	N	15	THR
4	N	23	ASP
4	N	30	ARG
4	N	42	HIS
4	N	57	SER
4	N	63	LEU
4	N	82	ASP
4	O	7	ASN
4	O	15	THR
4	O	17	GLU
4	O	22	VAL
4	O	23	ASP
4	O	30	ARG
4	O	42	HIS
4	O	46	GLU
4	O	51	THR
4	O	57	SER
4	O	63	LEU
4	O	72	VAL
4	O	81	SER
4	O	85	SER
4	P	7	ASN
4	P	15	THR
4	P	23	ASP
4	P	30	ARG
4	P	42	HIS
4	P	57	SER
4	P	63	LEU
4	P	82	ASP
4	P	85	SER
4	Q	7	ASN
4	Q	15	THR

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Mol	Chain	Res	Type
4	Q	23	ASP
4	Q	30	ARG
4	Q	42	HIS
4	Q	57	SER
4	Q	63	LEU
4	Q	82	ASP
4	Q	85	SER
4	R	7	ASN
4	R	15	THR
4	R	17	GLU
4	R	23	ASP
4	R	30	ARG
4	R	42	HIS
4	R	57	SER
4	R	63	LEU
4	R	82	ASP
4	R	85	SER
5	T	26	ARG
5	T	35	ASP
5	T	37	CYS
5	T	40	GLN
5	T	42	GLU
5	T	43	ARG
5	T	47	VAL
5	T	65	THR
5	T	71	HIS
5	T	72	ARG
5	T	76	GLU
5	T	82	ASP
5	T	98	VAL
5	T	99	SER
5	T	109	ASN
5	T	111	ASP
5	T	112	ASP
5	T	114	LEU
5	T	119	THR
5	T	123	ARG
5	T	124	ASP
5	T	126	ARG
5	T	154	VAL
5	T	162	VAL
5	T	163	THR

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Mol	Chain	Res	Type
5	T	164	GLN
5	T	171	THR
5	T	172	CYS
5	T	177	ASP
5	T	182	ARG
5	T	186	MET
5	T	198	CYS
5	T	205	ARG
5	T	206	GLU
5	T	213	ASP
5	T	225	THR
5	T	235	VAL
5	T	244	GLU
5	T	249	LEU
5	T	252	LEU
5	T	256	THR
5	T	265	THR
5	T	293	CYS
5	T	295	THR
5	T	298	LEU
5	T	299	ASN
5	T	300	THR
5	T	321	SER
4	V	7	ASN
4	V	15	THR
4	V	17	GLU
4	V	22	VAL
4	V	23	ASP
4	V	30	ARG
4	V	42	HIS
4	V	57	SER
4	V	63	LEU
4	V	82	ASP
4	V	85	SER
1	f	808	ARG
1	g	1269	LYS
5	h	37	CYS
5	h	40	GLN
5	h	42	GLU
5	h	43	ARG
5	h	47	VAL
5	h	71	HIS

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Mol	Chain	Res	Type
5	h	72	ARG
5	h	76	GLU
5	h	82	ASP
5	h	98	VAL
5	h	99	SER
5	h	109	ASN
5	h	111	ASP
5	h	112	ASP
5	h	114	LEU
5	h	119	THR
5	h	123	ARG
5	h	124	ASP
5	h	126	ARG
5	h	154	VAL
5	h	162	VAL
5	h	163	THR
5	h	164	GLN
5	h	171	THR
5	h	172	CYS
5	h	177	ASP
5	h	182	ARG
5	h	186	MET
5	h	198	CYS
5	h	205	ARG
5	h	206	GLU
5	h	213	ASP
5	h	225	THR
5	h	235	VAL
5	h	244	GLU
5	h	249	LEU
5	h	252	LEU
5	h	256	THR
5	h	265	THR
5	h	293	CYS
5	h	295	THR
5	h	298	LEU
5	h	300	THR
5	h	321	SER
5	i	35	ASP
5	i	37	CYS
5	i	40	GLN
5	i	42	GLU

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Mol	Chain	Res	Type
5	i	43	ARG
5	i	47	VAL
5	i	65	THR
5	i	71	HIS
5	i	72	ARG
5	i	76	GLU
5	i	82	ASP
5	i	98	VAL
5	i	99	SER
5	i	109	ASN
5	i	111	ASP
5	i	112	ASP
5	i	114	LEU
5	i	119	THR
5	i	123	ARG
5	i	124	ASP
5	i	126	ARG
5	i	154	VAL
5	i	162	VAL
5	i	163	THR
5	i	164	GLN
5	i	171	THR
5	i	172	CYS
5	i	177	ASP
5	i	182	ARG
5	i	186	MET
5	i	198	CYS
5	i	205	ARG
5	i	206	GLU
5	i	225	THR
5	i	235	VAL
5	i	244	GLU
5	i	249	LEU
5	i	252	LEU
5	i	256	THR
5	i	265	THR
5	i	293	CYS
5	i	295	THR
5	i	298	LEU
5	i	299	ASN
5	i	300	THR
5	i	321	SER

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Mol	Chain	Res	Type
2	j	44	CYS
1	m	1245	ARG
1	q	1167	ARG
5	r	26	ARG
5	r	35	ASP
5	r	37	CYS
5	r	40	GLN
5	r	42	GLU
5	r	43	ARG
5	r	47	VAL
5	r	65	THR
5	r	71	HIS
5	r	72	ARG
5	r	76	GLU
5	r	82	ASP
5	r	98	VAL
5	r	99	SER
5	r	109	ASN
5	r	111	ASP
5	r	112	ASP
5	r	114	LEU
5	r	119	THR
5	r	123	ARG
5	r	124	ASP
5	r	126	ARG
5	r	154	VAL
5	r	162	VAL
5	r	163	THR
5	r	164	GLN
5	r	171	THR
5	r	172	CYS
5	r	177	ASP
5	r	182	ARG
5	r	186	MET
5	r	198	CYS
5	r	205	ARG
5	r	206	GLU
5	r	213	ASP
5	r	225	THR
5	r	235	VAL
5	r	244	GLU
5	r	249	LEU

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Mol	Chain	Res	Type
5	r	252	LEU
5	r	256	THR
5	r	265	THR
5	r	293	CYS
5	r	295	THR
5	r	298	LEU
5	r	299	ASN
5	r	300	THR
5	r	321	SER
5	t	26	ARG
5	t	35	ASP
5	t	37	CYS
5	t	40	GLN
5	t	42	GLU
5	t	43	ARG
5	t	47	VAL
5	t	65	THR
5	t	71	HIS
5	t	72	ARG
5	t	76	GLU
5	t	82	ASP
5	t	98	VAL
5	t	99	SER
5	t	109	ASN
5	t	111	ASP
5	t	112	ASP
5	t	114	LEU
5	t	119	THR
5	t	123	ARG
5	t	124	ASP
5	t	126	ARG
5	t	154	VAL
5	t	162	VAL
5	t	163	THR
5	t	164	GLN
5	t	171	THR
5	t	172	CYS
5	t	177	ASP
5	t	182	ARG
5	t	186	MET
5	t	198	CYS
5	t	205	ARG

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Mol	Chain	Res	Type
5	t	206	GLU
5	t	213	ASP
5	t	225	THR
5	t	235	VAL
5	t	244	GLU
5	t	249	LEU
5	t	252	LEU
5	t	256	THR
5	t	265	THR
5	t	293	CYS
5	t	295	THR
5	t	298	LEU
5	t	299	ASN
5	t	300	THR
5	t	321	SER
2	v	20	ARG
2	x	44	CYS
1	y	1132	PHE
1	y	1136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (451) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	136	ASN
1	0	277	HIS
1	0	286	HIS
1	0	397	HIS
1	0	434	HIS
1	0	441	HIS
1	0	512	ASN
1	0	556	ASN
1	0	692	ASN
1	0	693	GLN
1	0	700	HIS
1	0	734	ASN
1	0	769	GLN
1	0	835	HIS
1	0	850	ASN
1	0	864	GLN
1	0	898	HIS
1	0	904	HIS
1	0	938	HIS

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Mol	Chain	Res	Type
1	0	961	HIS
1	0	966	ASN
1	0	987	ASN
1	0	1096	GLN
1	0	1189	HIS
1	0	1191	HIS
1	0	1203	ASN
1	0	1309	HIS
2	1	88	GLN
2	1	176	ASN
2	1	187	ASN
2	2	19	GLN
2	2	34	HIS
2	2	205	ASN
2	2	217	ASN
2	3	89	ASN
2	3	132	GLN
2	3	176	ASN
2	3	205	ASN
2	3	235	GLN
2	3	242	GLN
1	A	19	HIS
1	A	36	ASN
1	A	89	GLN
1	A	103	GLN
1	A	277	HIS
1	A	286	HIS
1	A	375	ASN
1	A	413	HIS
1	A	434	HIS
1	A	441	HIS
1	A	456	GLN
1	A	482	GLN
1	A	556	ASN
1	A	579	HIS
1	A	674	HIS
1	A	700	HIS
1	A	775	HIS
1	A	835	HIS
1	A	838	ASN
1	A	849	HIS
1	A	850	ASN

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Mol	Chain	Res	Type
1	A	869	ASN
1	A	912	GLN
1	A	973	GLN
1	A	978	HIS
1	A	987	ASN
1	A	1096	GLN
1	A	1191	HIS
1	A	1198	HIS
1	A	1203	ASN
1	A	1208	GLN
3	B	4	HIS
3	B	44	HIS
3	B	46	GLN
3	B	50	HIS
3	B	143	GLN
3	B	163	HIS
3	B	301	HIS
3	B	317	GLN
3	B	532	GLN
3	B	542	HIS
4	F	67	HIS
4	G	29	ASN
4	H	29	ASN
4	I	29	ASN
4	J	67	HIS
4	K	29	ASN
4	N	29	ASN
4	R	29	ASN
1	S	99	HIS
1	S	136	ASN
1	S	172	GLN
1	S	277	HIS
1	S	278	HIS
1	S	413	HIS
1	S	434	HIS
1	S	441	HIS
1	S	462	GLN
1	S	506	GLN
1	S	556	ASN
1	S	579	HIS
1	S	650	ASN
1	S	692	ASN

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Mol	Chain	Res	Type
1	S	693	GLN
1	S	700	HIS
1	S	734	ASN
1	S	739	GLN
1	S	835	HIS
1	S	838	ASN
1	S	904	HIS
1	S	914	ASN
1	S	938	HIS
1	S	987	ASN
1	S	1008	GLN
1	S	1064	GLN
1	S	1148	GLN
1	S	1180	HIS
5	T	53	HIS
5	T	194	HIS
5	T	260	ASN
5	T	263	HIS
1	U	89	GLN
1	U	227	ASN
1	U	253	HIS
1	U	434	HIS
1	U	441	HIS
1	U	556	ASN
1	U	628	GLN
1	U	650	ASN
1	U	693	GLN
1	U	740	HIS
1	U	832	HIS
1	U	835	HIS
1	U	845	ASN
1	U	869	ASN
1	U	904	HIS
1	U	973	GLN
1	U	977	GLN
1	U	1008	GLN
1	U	1121	ASN
1	U	1210	HIS
1	U	1309	HIS
4	V	29	ASN
1	a	103	GLN
1	a	106	HIS

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Mol	Chain	Res	Type
1	a	172	GLN
1	a	253	HIS
1	a	375	ASN
1	a	434	HIS
1	a	441	HIS
1	a	462	GLN
1	a	610	HIS
1	a	635	HIS
1	a	636	ASN
1	a	750	ASN
1	a	772	HIS
1	a	832	HIS
1	a	842	ASN
1	a	938	HIS
1	a	955	HIS
1	a	961	HIS
1	a	977	GLN
1	a	987	ASN
1	a	1059	HIS
1	a	1147	GLN
1	a	1198	HIS
1	a	1312	GLN
1	e	106	HIS
1	e	286	HIS
1	e	482	GLN
1	e	512	ASN
1	e	610	HIS
1	e	635	HIS
1	e	740	HIS
1	e	761	ASN
1	e	903	HIS
1	e	978	HIS
1	e	987	ASN
1	e	1014	HIS
1	f	21	HIS
1	f	106	HIS
1	f	253	HIS
1	f	302	ASN
1	f	434	HIS
1	f	441	HIS
1	f	556	ASN
1	f	672	HIS

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Mol	Chain	Res	Type
1	f	674	HIS
1	f	692	ASN
1	f	693	GLN
1	f	811	GLN
1	f	814	GLN
1	f	864	GLN
1	f	898	HIS
1	f	903	HIS
1	f	955	HIS
1	f	987	ASN
1	f	1012	GLN
1	f	1203	ASN
1	f	1309	HIS
1	g	19	HIS
1	g	136	ASN
1	g	278	HIS
1	g	300	ASN
1	g	419	HIS
1	g	434	HIS
1	g	462	GLN
1	g	554	ASN
1	g	579	HIS
1	g	610	HIS
1	g	695	GLN
1	g	700	HIS
1	g	748	GLN
1	g	769	GLN
1	g	798	ASN
1	g	811	GLN
1	g	832	HIS
1	g	930	ASN
1	g	1014	HIS
1	g	1124	ASN
1	g	1203	ASN
1	g	1210	HIS
5	h	53	HIS
5	h	194	HIS
5	h	260	ASN
5	h	263	HIS
5	i	53	HIS
5	i	194	HIS
5	i	260	ASN

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Mol	Chain	Res	Type
5	i	263	HIS
2	j	69	HIS
2	j	97	ASN
2	k	88	GLN
2	k	168	GLN
2	k	231	GLN
1	l	21	HIS
1	l	157	ASN
1	l	172	GLN
1	l	253	HIS
1	l	434	HIS
1	l	441	HIS
1	l	462	GLN
1	l	597	ASN
1	l	642	ASN
1	l	700	HIS
1	l	761	ASN
1	l	772	HIS
1	l	798	ASN
1	l	835	HIS
1	l	864	GLN
1	l	869	ASN
1	l	898	HIS
1	l	903	HIS
1	l	904	HIS
1	l	938	HIS
1	l	954	GLN
1	l	966	ASN
1	l	987	ASN
1	l	1008	GLN
1	l	1203	ASN
1	l	1312	GLN
1	m	21	HIS
1	m	85	GLN
1	m	153	GLN
1	m	172	GLN
1	m	302	ASN
1	m	434	HIS
1	m	556	ASN
1	m	610	HIS
1	m	692	ASN
1	m	734	ASN

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Mol	Chain	Res	Type
1	m	740	HIS
1	m	811	GLN
1	m	814	GLN
1	m	835	HIS
1	m	845	ASN
1	m	869	ASN
1	m	914	ASN
1	m	938	HIS
1	m	966	ASN
1	m	978	HIS
1	m	1121	ASN
1	m	1198	HIS
1	m	1203	ASN
1	m	1309	HIS
1	n	90	GLN
1	n	106	HIS
1	n	159	GLN
1	n	172	GLN
1	n	253	HIS
1	n	302	ASN
1	n	434	HIS
1	n	441	HIS
1	n	672	HIS
1	n	674	HIS
1	n	693	GLN
1	n	695	GLN
1	n	740	HIS
1	n	811	GLN
1	n	835	HIS
1	n	850	ASN
1	n	904	HIS
1	n	977	GLN
1	n	978	HIS
1	n	1097	ASN
1	n	1121	ASN
1	n	1203	ASN
1	n	1309	HIS
2	o	163	ASN
2	o	242	GLN
1	p	253	HIS
1	p	273	GLN
1	p	302	ASN

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Mol	Chain	Res	Type
1	p	367	GLN
1	p	375	ASN
1	p	434	HIS
1	p	441	HIS
1	p	462	GLN
1	p	579	HIS
1	p	628	GLN
1	p	672	HIS
1	p	739	GLN
1	p	740	HIS
1	p	760	HIS
1	p	798	ASN
1	p	835	HIS
1	p	842	ASN
1	p	850	ASN
1	p	904	HIS
1	p	977	GLN
1	p	987	ASN
1	p	1121	ASN
1	p	1203	ASN
1	p	1208	GLN
1	p	1309	HIS
1	q	441	HIS
1	q	482	GLN
1	q	506	GLN
1	q	541	GLN
1	q	579	HIS
1	q	597	ASN
1	q	610	HIS
1	q	700	HIS
1	q	737	HIS
1	q	775	HIS
1	q	814	GLN
1	q	835	HIS
1	q	842	ASN
1	q	849	HIS
1	q	904	HIS
1	q	938	HIS
1	q	966	ASN
1	q	978	HIS
1	q	1012	GLN
1	q	1014	HIS

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Mol	Chain	Res	Type
1	q	1064	GLN
1	q	1121	ASN
1	q	1220	GLN
1	q	1309	HIS
5	r	53	HIS
5	r	194	HIS
5	r	260	ASN
5	r	263	HIS
2	s	34	HIS
2	s	69	HIS
2	s	88	GLN
2	s	242	GLN
5	t	53	HIS
5	t	194	HIS
5	t	260	ASN
5	t	263	HIS
1	u	11	GLN
1	u	90	GLN
1	u	136	ASN
1	u	159	GLN
1	u	273	GLN
1	u	302	ASN
1	u	441	HIS
1	u	610	HIS
1	u	693	GLN
1	u	740	HIS
1	u	769	GLN
1	u	798	ASN
1	u	835	HIS
1	u	850	ASN
1	u	864	GLN
1	u	904	HIS
1	u	938	HIS
1	u	955	HIS
1	u	961	HIS
1	u	966	ASN
1	u	1121	ASN
1	u	1191	HIS
2	v	69	HIS
2	v	231	GLN
1	w	36	ASN
1	w	37	ASN

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Mol	Chain	Res	Type
1	w	253	HIS
1	w	277	HIS
1	w	397	HIS
1	w	434	HIS
1	w	482	GLN
1	w	628	GLN
1	w	635	HIS
1	w	636	ASN
1	w	642	ASN
1	w	672	HIS
1	w	693	GLN
1	w	700	HIS
1	w	740	HIS
1	w	835	HIS
1	w	850	ASN
1	w	869	ASN
1	w	904	HIS
1	w	914	ASN
1	w	1134	GLN
1	w	1189	HIS
1	w	1196	HIS
1	w	1309	HIS
1	w	1312	GLN
2	x	69	HIS
2	x	97	ASN
2	x	119	ASN
2	x	193	ASN
2	x	231	GLN
1	y	172	GLN
1	y	277	HIS
1	y	434	HIS
1	y	441	HIS
1	y	541	GLN
1	y	579	HIS
1	y	699	ASN
1	y	740	HIS
1	y	798	ASN
1	y	835	HIS
1	y	845	ASN
1	y	850	ASN
1	y	864	GLN
1	y	869	ASN

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Mol	Chain	Res	Type
1	y	914	ASN
1	y	1008	GLN
1	y	1012	GLN
1	y	1014	HIS
1	y	1121	ASN
1	y	1210	HIS
1	y	1286	GLN
1	y	1309	HIS
2	z	132	GLN
2	z	193	ASN
2	z	231	GLN
2	z	242	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

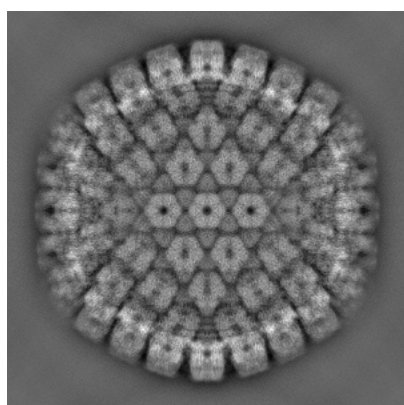
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31611. These allow visual inspection of the internal detail of the map and identification of artifacts.

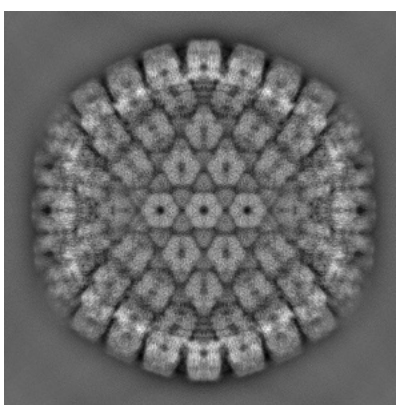
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

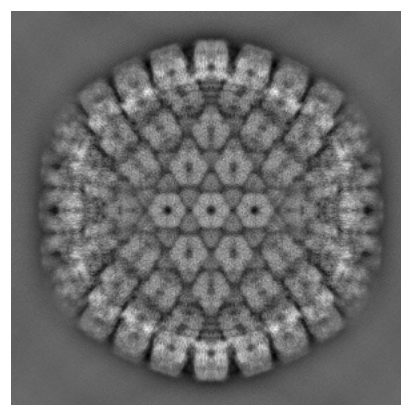
6.1.1 Primary map



X



Y

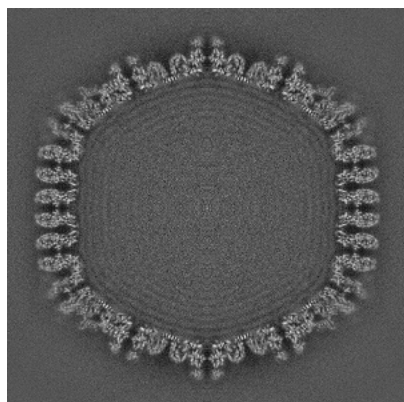


Z

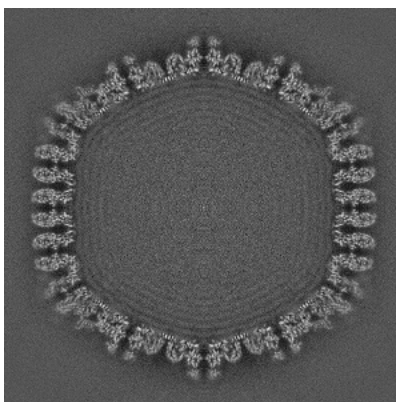
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

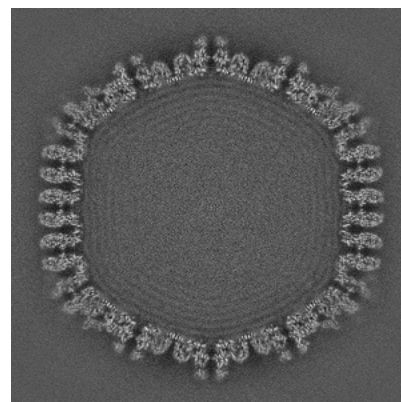
6.2.1 Primary map



X Index: 640



Y Index: 640

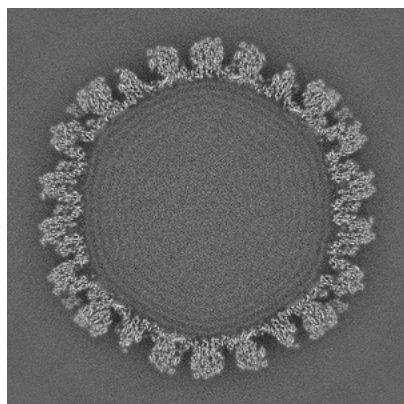


Z Index: 640

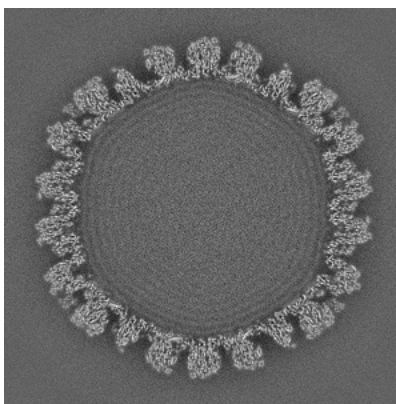
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

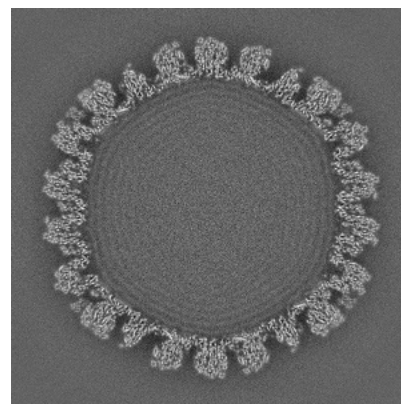
6.3.1 Primary map



X Index: 750



Y Index: 750

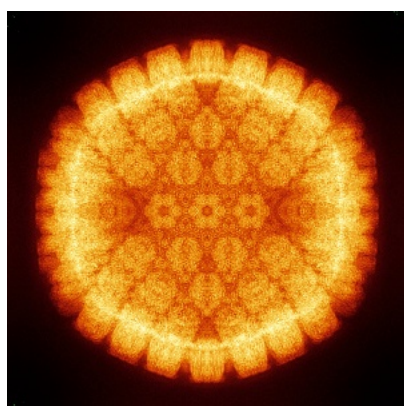


Z Index: 529

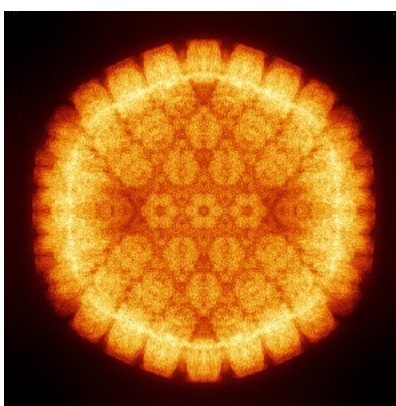
The images above show the largest variance slices of the map in three orthogonal directions.

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

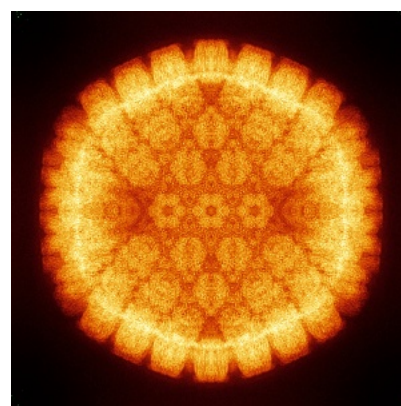
6.4.1 Primary map



X



Y

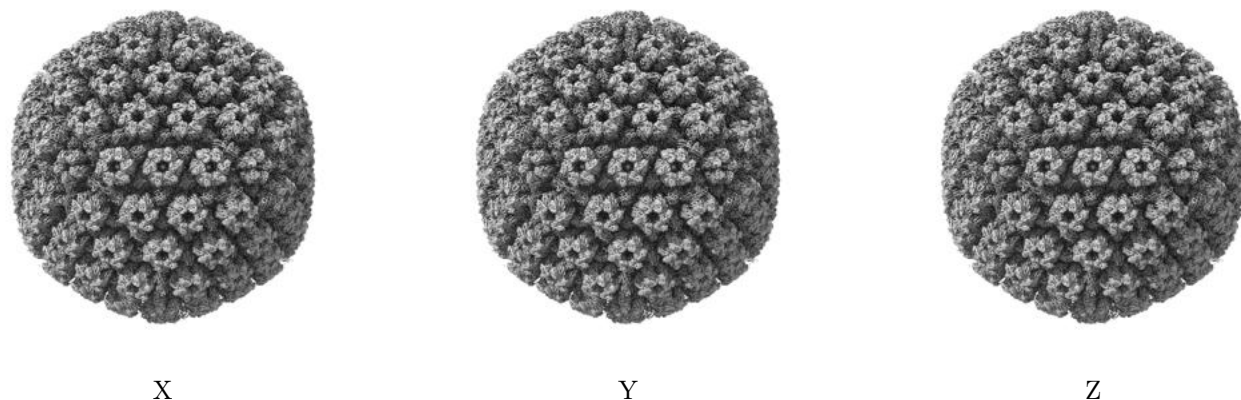


Z

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 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

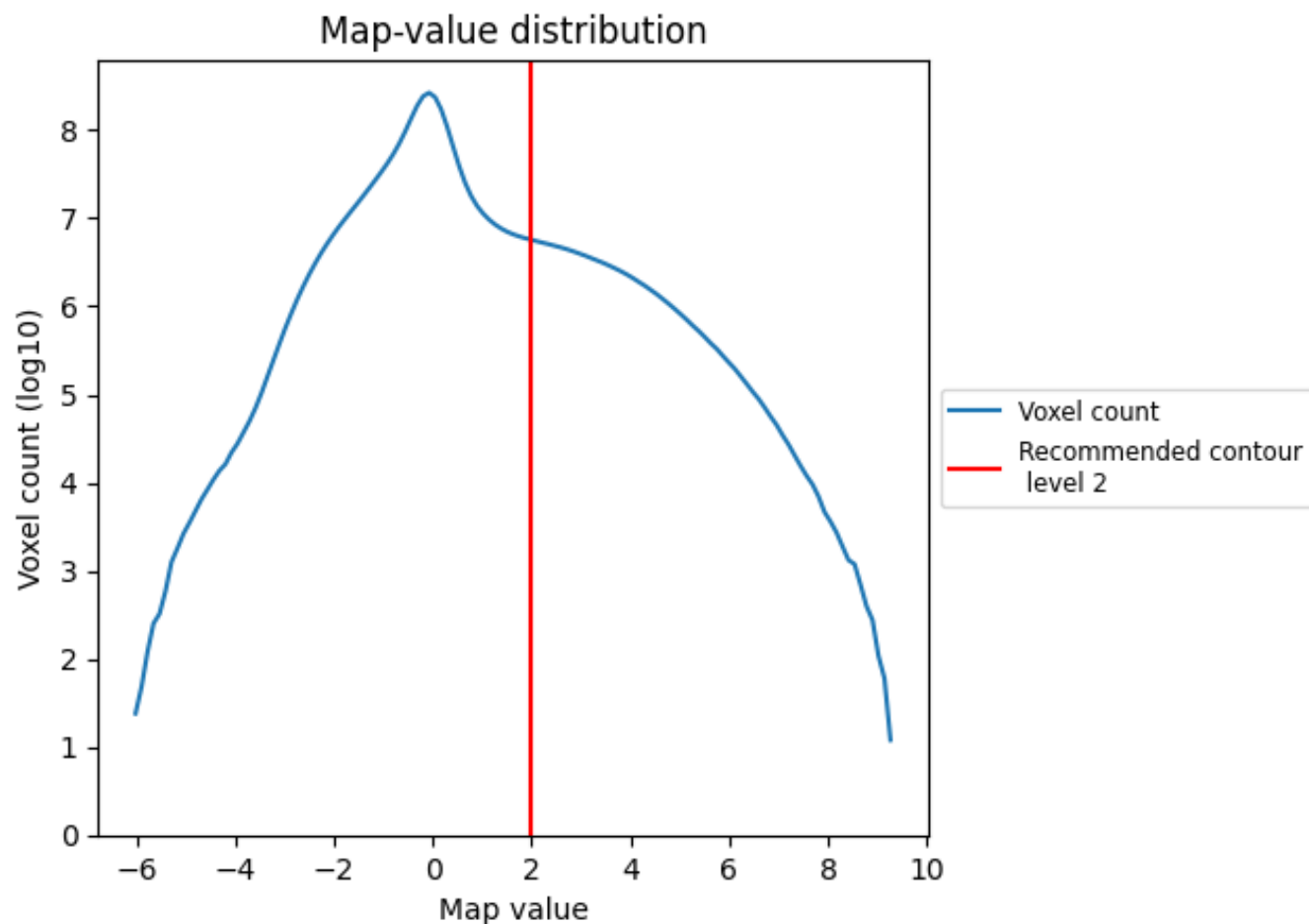
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

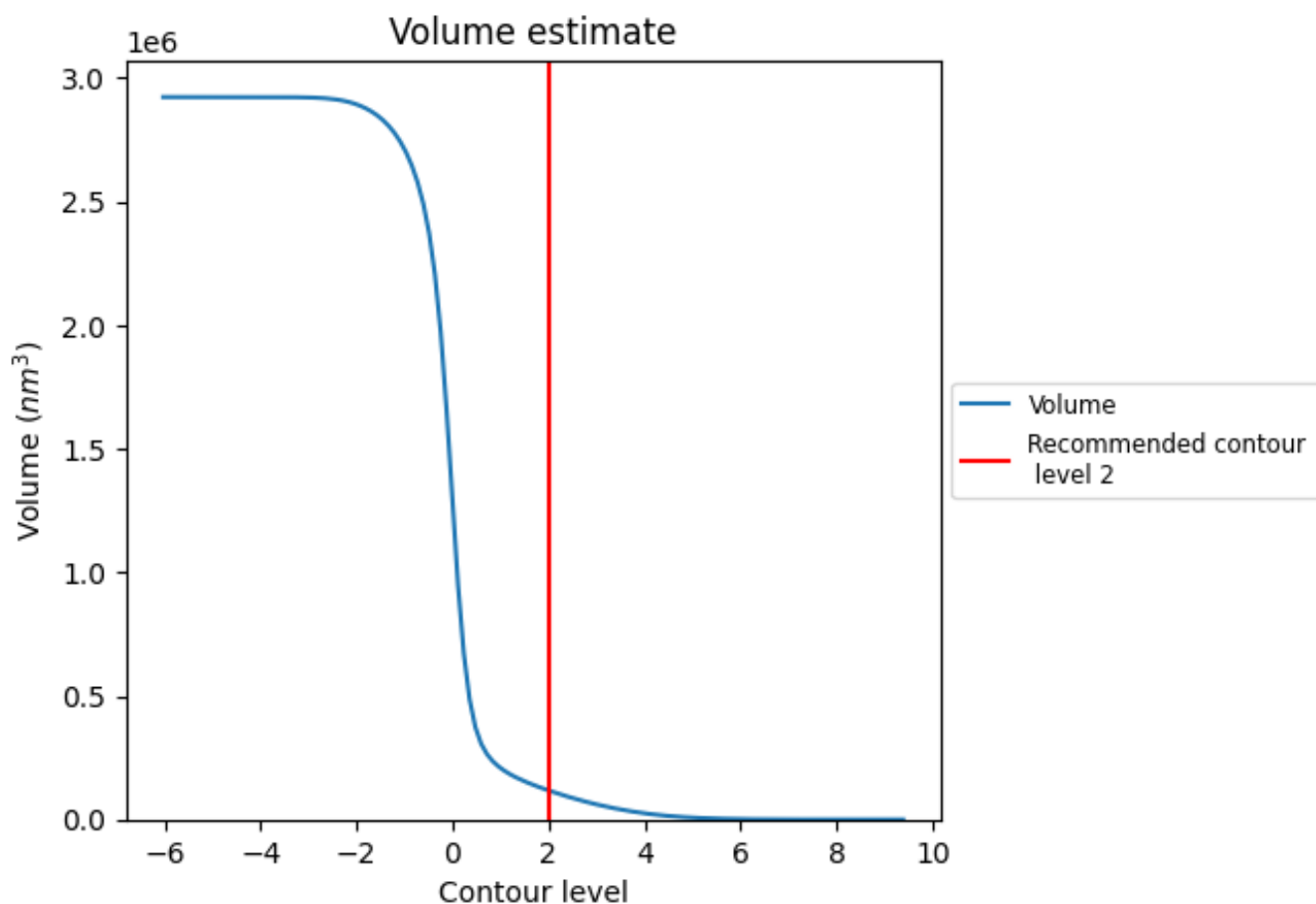
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

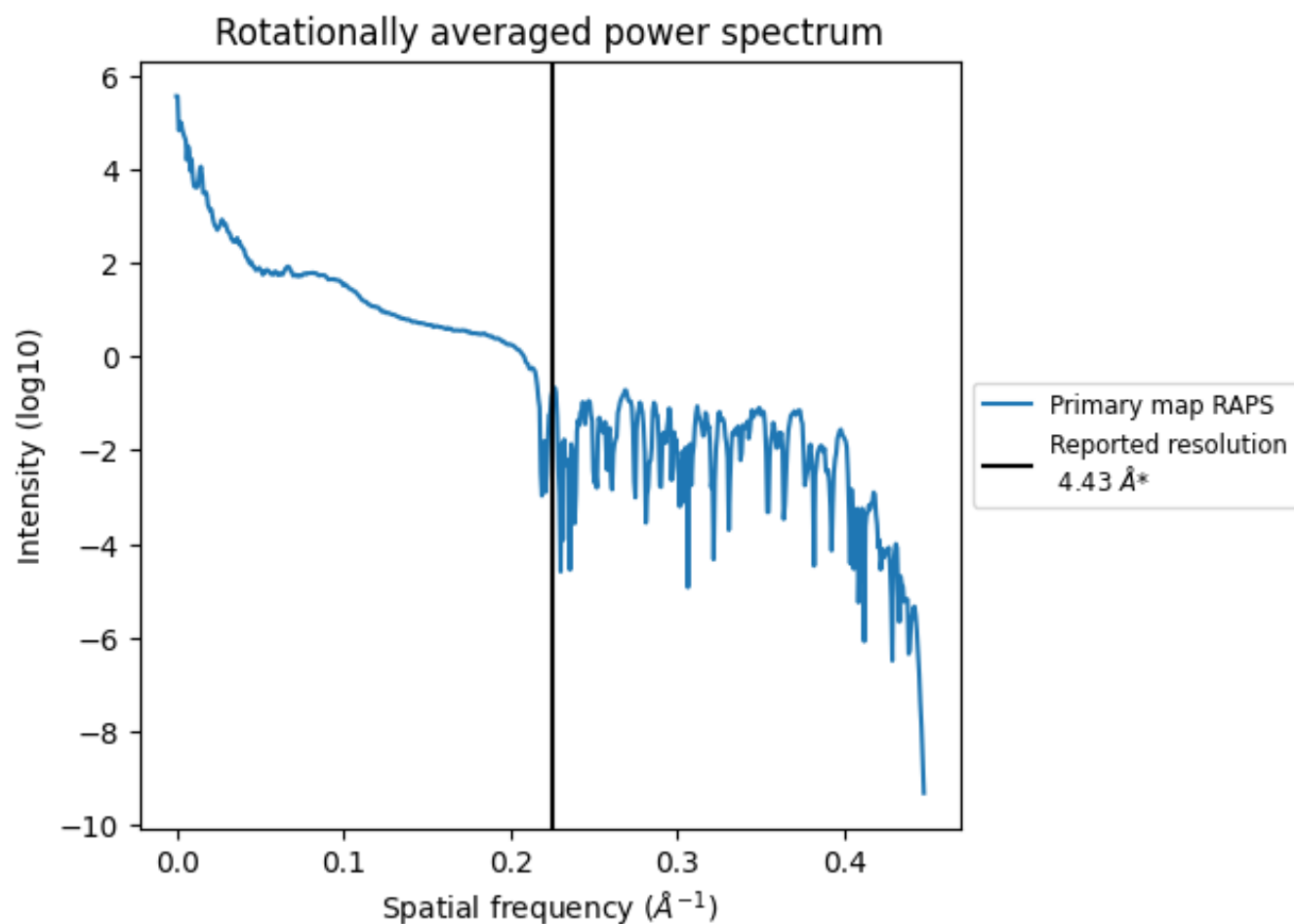
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117685 nm³; this corresponds to an approximate mass of 106308 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 0.226 Å⁻¹

8 Fourier-Shell correlation

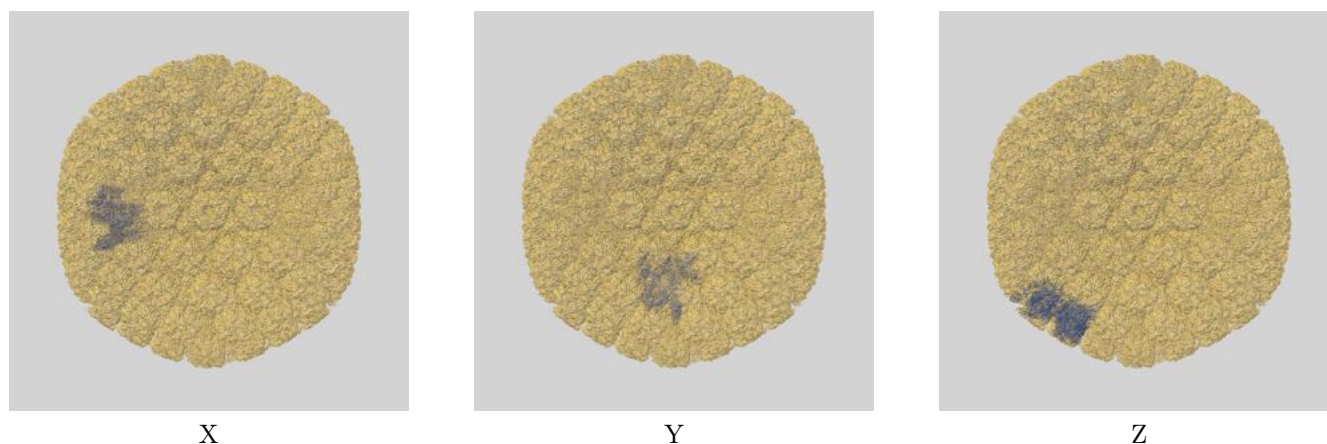
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

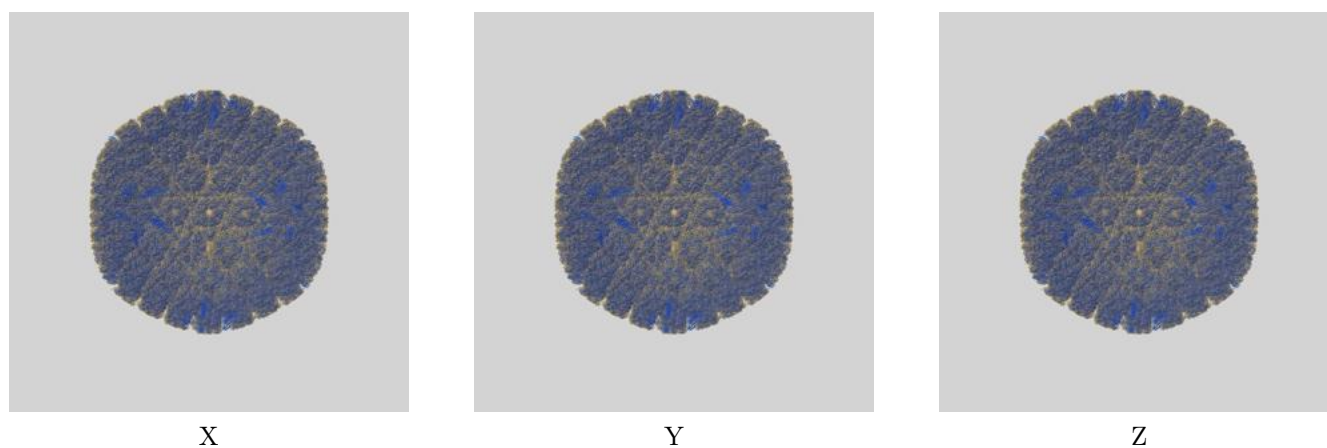
This section contains information regarding the fit between EMDB map EMD-31611 and PDB model 7FJ1. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

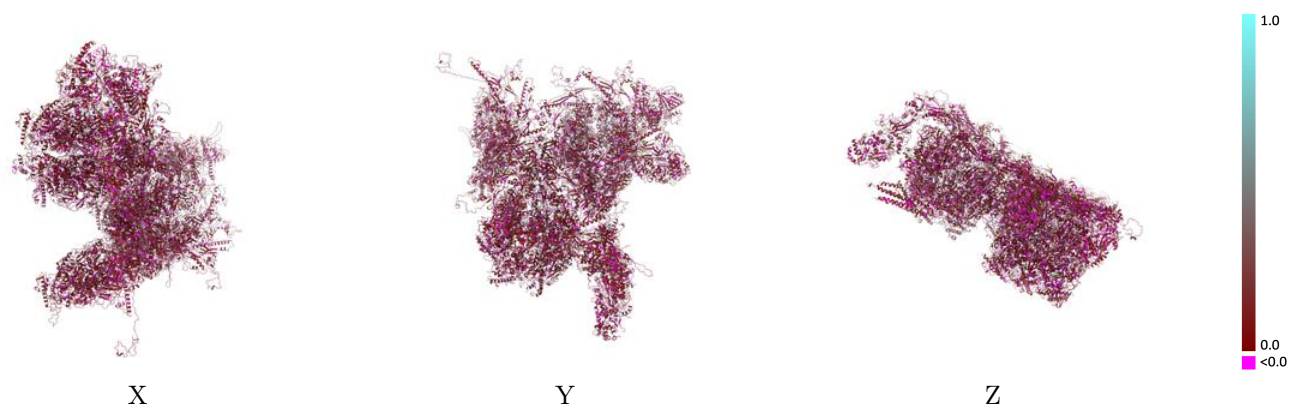


9.1.2 Map-model assembly overlay [i](#)



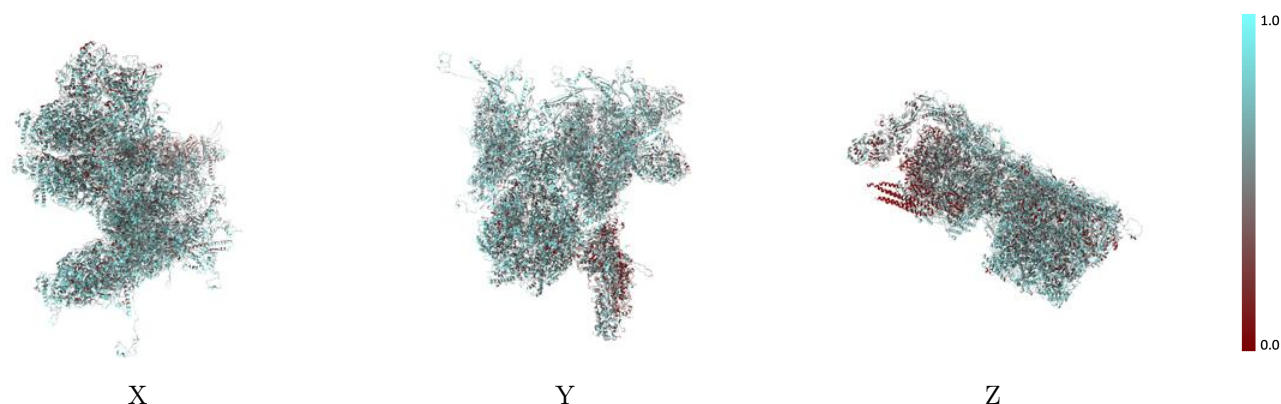
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



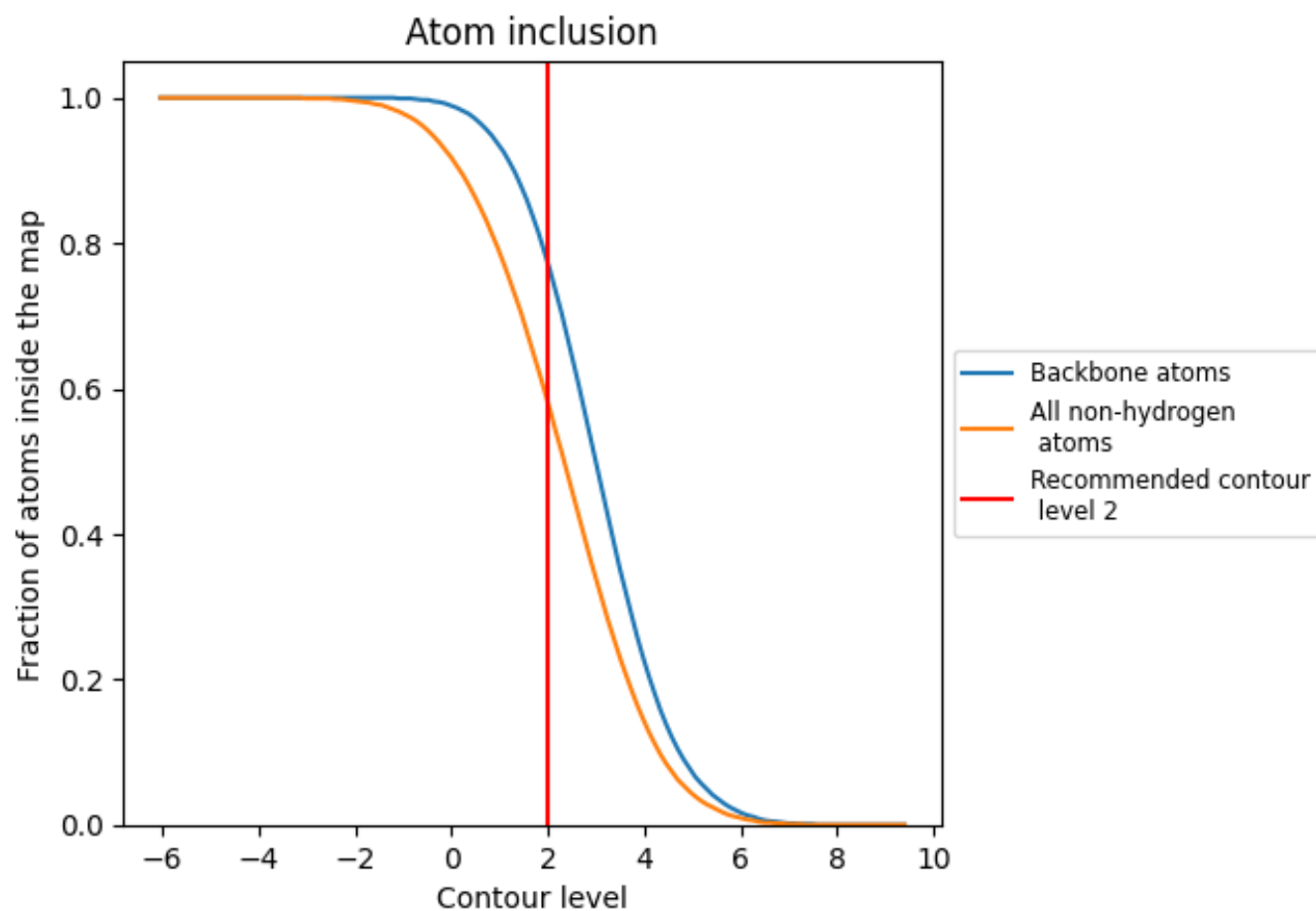
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5810	 0.1420
0	 0.6010	 0.1380
1	 0.5760	 0.1580
2	 0.5600	 0.1460
3	 0.5650	 0.1330
A	 0.6230	 0.1420
B	 0.1850	 0.1400
E	 0.6680	 0.1500
F	 0.6750	 0.1480
G	 0.6800	 0.1350
H	 0.6800	 0.1420
I	 0.6060	 0.1580
J	 0.6690	 0.1530
K	 0.6950	 0.1700
L	 0.6630	 0.1610
M	 0.7030	 0.1710
N	 0.6760	 0.1590
O	 0.6150	 0.1490
P	 0.6760	 0.1820
Q	 0.7220	 0.1670
R	 0.6620	 0.1600
S	 0.5820	 0.1450
T	 0.5940	 0.1400
U	 0.6080	 0.1450
V	 0.6400	 0.1450
X	 0.1330	 0.1370
Y	 0.1220	 0.1220
Z	 0.0550	 0.0980
a	 0.5870	 0.1370
c	 0.2060	 0.1530
e	 0.4760	 0.1350
f	 0.6240	 0.1460
g	 0.6070	 0.1440
h	 0.6340	 0.1690
i	 0.3910	 0.1260



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Chain	Atom inclusion	Q-score
j	 0.3620	 0.1500
k	 0.3820	 0.1550
l	 0.6030	 0.1430
m	 0.6150	 0.1380
n	 0.6030	 0.1360
o	 0.5490	 0.1580
p	 0.6080	 0.1440
q	 0.6000	 0.1400
r	 0.5780	 0.1310
s	 0.5790	 0.1550
t	 0.5590	 0.1180
u	 0.6260	 0.1480
v	 0.5680	 0.1420
w	 0.5980	 0.1420
x	 0.5280	 0.1360
y	 0.6200	 0.1400
z	 0.5370	 0.1330