



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:51 AM UTC

PDB ID : 9SCW / pdb\_00009scw  
Title : Crystal structure of Coxsackie B1 virus-like particle delta-palxa  
Authors : Haikarainen, T.  
Deposited on : 2025-08-12  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

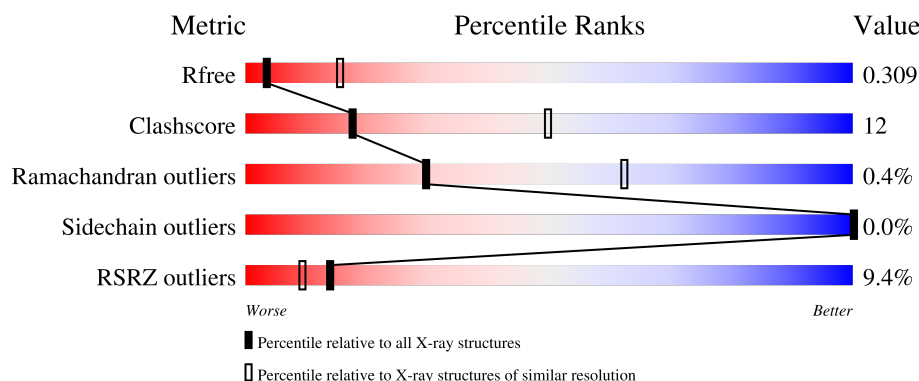
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	263	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>
1	1	263	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>24%</div> <div>15%</div> </div> </div>
1	8	263	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>17%</div> </div> </div>
1	A	263	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>13%</div> </div> </div>
1	AC	263	<div> <div>10%</div> <div> <div></div> <div>56%</div> <div>27%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	AG	263	
1	AK	263	
1	AO	263	
1	E	263	
1	I	263	
1	M	263	
1	Q	263	
1	U	263	
1	Y	263	
1	c	263	
1	g	263	
1	k	263	
1	o	263	
1	s	263	
1	w	263	
2	2	263	
2	5	263	
2	9	263	
2	AD	263	
2	AH	263	
2	AL	263	
2	AP	263	
2	B	263	
2	F	263	
2	J	263	

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Mol	Chain	Length	Quality of chain
2	N	263	
2	R	263	
2	V	263	
2	Z	263	
2	d	263	
2	h	263	
2	l	263	
2	p	263	
2	t	263	
2	x	263	
3	3	238	
3	6	238	
3	AA	238	
3	AE	238	
3	AI	238	
3	AM	238	
3	AQ	238	
3	C	238	
3	G	238	
3	K	238	
3	O	238	
3	S	238	
3	W	238	
3	a	238	
3	e	238	

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Mol	Chain	Length	Quality of chain
3	i	238	
3	m	238	
3	q	238	
3	u	238	
3	y	238	
4	4	69	
4	D	69	
4	H	69	
4	L	69	
4	P	69	
4	T	69	
4	X	69	
4	b	69	
4	f	69	
4	j	69	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 211656 atoms, of which 103219 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1	223	Total	C	H	N	O	S	0	0	0
			3472	1125	1709	304	326	8			
1	A	228	Total	C	H	N	O	S	0	0	0
			3546	1153	1736	314	335	8			
1	E	222	Total	C	H	N	O	S	0	0	0
			3479	1126	1712	306	327	8			
1	Y	221	Total	C	H	N	O	S	0	0	0
			3493	1126	1728	305	326	8			
1	g	222	Total	C	H	N	O	S	0	0	0
			3495	1129	1724	307	327	8			
1	I	223	Total	C	H	N	O	S	0	0	0
			3493	1129	1722	306	328	8			
1	M	222	Total	C	H	N	O	S	0	0	0
			3481	1126	1714	306	327	8			
1	Q	222	Total	C	H	N	O	S	0	0	0
			3494	1129	1723	307	327	8			
1	U	222	Total	C	H	N	O	S	0	0	0
			3479	1126	1712	306	327	8			
1	c	222	Total	C	H	N	O	S	0	0	0
			3480	1126	1713	306	327	8			
1	k	218	Total	C	H	N	O	S	0	0	0
			3334	1091	1627	290	318	8			
1	o	218	Total	C	H	N	O	S	0	0	0
			3359	1093	1649	294	315	8			
1	s	219	Total	C	H	N	O	S	0	0	0
			3352	1093	1640	294	317	8			
1	w	221	Total	C	H	N	O	S	0	0	0
			3304	1089	1600	287	320	8			
1	0	217	Total	C	H	N	O	S	0	0	0
			3301	1080	1612	288	313	8			
1	8	218	Total	C	H	N	O	S	0	0	0
			3230	1063	1566	284	309	8			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AC	219	Total	C	H	N	O	S	0	0	0
			3296	1081	1603	289	315	8			
1	AG	219	Total	C	H	N	O	S	0	0	0
			3274	1079	1586	285	316	8			
1	AK	219	Total	C	H	N	O	S	0	0	0
			3287	1080	1599	286	314	8			
1	AO	219	Total	C	H	N	O	S	0	0	0
			3265	1076	1580	285	316	8			

There are 560 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	21	ARG	LYS	conflict	UNP P08291
1	?	-	SER	deletion	UNP P08291
1	?	-	GLU	deletion	UNP P08291
1	?	-	SER	deletion	UNP P08291
1	?	-	ILE	deletion	UNP P08291
1	?	-	PRO	deletion	UNP P08291
1	?	-	ALA	deletion	UNP P08291
1	?	-	LEU	deletion	UNP P08291
1	?	-	THR	deletion	UNP P08291
1	?	-	ALA	deletion	UNP P08291
1	?	-	ALA	deletion	UNP P08291
1	?	-	GLU	deletion	UNP P08291
1	?	-	THR	deletion	UNP P08291
1	?	-	GLY	deletion	UNP P08291
1	?	-	HIS	deletion	UNP P08291
1	?	-	THR	deletion	UNP P08291
1	56	ALA	SER	conflict	UNP P08291
1	65	THR	ASN	conflict	UNP P08291
1	86	ARG	LEU	conflict	UNP P08291
1	88	LYS	ARG	conflict	UNP P08291
1	89	LEU	LYS	conflict	UNP P08291
1	90	GLU	LEU	conflict	UNP P08291
1	91	LEU	GLU	conflict	UNP P08291
1	110	GLN	GLU	conflict	UNP P08291
1	124	HIS	GLN	conflict	UNP P08291
1	249	THR	ASN	conflict	UNP P08291
1	258	VAL	SER	conflict	UNP P08291
1	259	GLY	ASN	conflict	UNP P08291
A	21	ARG	LYS	conflict	UNP P08291
A	?	-	SER	deletion	UNP P08291
A	?	-	GLU	deletion	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P08291
A	?	-	ILE	deletion	UNP P08291
A	?	-	PRO	deletion	UNP P08291
A	?	-	ALA	deletion	UNP P08291
A	?	-	LEU	deletion	UNP P08291
A	?	-	THR	deletion	UNP P08291
A	?	-	ALA	deletion	UNP P08291
A	?	-	ALA	deletion	UNP P08291
A	?	-	GLU	deletion	UNP P08291
A	?	-	THR	deletion	UNP P08291
A	?	-	GLY	deletion	UNP P08291
A	?	-	HIS	deletion	UNP P08291
A	?	-	THR	deletion	UNP P08291
A	56	ALA	SER	conflict	UNP P08291
A	65	THR	ASN	conflict	UNP P08291
A	86	ARG	LEU	conflict	UNP P08291
A	88	LYS	ARG	conflict	UNP P08291
A	89	LEU	LYS	conflict	UNP P08291
A	90	GLU	LEU	conflict	UNP P08291
A	91	LEU	GLU	conflict	UNP P08291
A	110	GLN	GLU	conflict	UNP P08291
A	124	HIS	GLN	conflict	UNP P08291
A	249	THR	ASN	conflict	UNP P08291
A	258	VAL	SER	conflict	UNP P08291
A	259	GLY	ASN	conflict	UNP P08291
E	21	ARG	LYS	conflict	UNP P08291
E	?	-	SER	deletion	UNP P08291
E	?	-	GLU	deletion	UNP P08291
E	?	-	SER	deletion	UNP P08291
E	?	-	ILE	deletion	UNP P08291
E	?	-	PRO	deletion	UNP P08291
E	?	-	ALA	deletion	UNP P08291
E	?	-	LEU	deletion	UNP P08291
E	?	-	THR	deletion	UNP P08291
E	?	-	ALA	deletion	UNP P08291
E	?	-	ALA	deletion	UNP P08291
E	?	-	GLU	deletion	UNP P08291
E	?	-	THR	deletion	UNP P08291
E	?	-	GLY	deletion	UNP P08291
E	?	-	HIS	deletion	UNP P08291
E	?	-	THR	deletion	UNP P08291
E	56	ALA	SER	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
E	65	THR	ASN	conflict	UNP P08291
E	86	ARG	LEU	conflict	UNP P08291
E	88	LYS	ARG	conflict	UNP P08291
E	89	LEU	LYS	conflict	UNP P08291
E	90	GLU	LEU	conflict	UNP P08291
E	91	LEU	GLU	conflict	UNP P08291
E	110	GLN	GLU	conflict	UNP P08291
E	124	HIS	GLN	conflict	UNP P08291
E	249	THR	ASN	conflict	UNP P08291
E	258	VAL	SER	conflict	UNP P08291
E	259	GLY	ASN	conflict	UNP P08291
Y	21	ARG	LYS	conflict	UNP P08291
Y	?	-	SER	deletion	UNP P08291
Y	?	-	GLU	deletion	UNP P08291
Y	?	-	SER	deletion	UNP P08291
Y	?	-	ILE	deletion	UNP P08291
Y	?	-	PRO	deletion	UNP P08291
Y	?	-	ALA	deletion	UNP P08291
Y	?	-	LEU	deletion	UNP P08291
Y	?	-	THR	deletion	UNP P08291
Y	?	-	ALA	deletion	UNP P08291
Y	?	-	ALA	deletion	UNP P08291
Y	?	-	GLU	deletion	UNP P08291
Y	?	-	THR	deletion	UNP P08291
Y	?	-	GLY	deletion	UNP P08291
Y	?	-	HIS	deletion	UNP P08291
Y	?	-	THR	deletion	UNP P08291
Y	56	ALA	SER	conflict	UNP P08291
Y	65	THR	ASN	conflict	UNP P08291
Y	86	ARG	LEU	conflict	UNP P08291
Y	88	LYS	ARG	conflict	UNP P08291
Y	89	LEU	LYS	conflict	UNP P08291
Y	90	GLU	LEU	conflict	UNP P08291
Y	91	LEU	GLU	conflict	UNP P08291
Y	110	GLN	GLU	conflict	UNP P08291
Y	124	HIS	GLN	conflict	UNP P08291
Y	249	THR	ASN	conflict	UNP P08291
Y	258	VAL	SER	conflict	UNP P08291
Y	259	GLY	ASN	conflict	UNP P08291
g	21	ARG	LYS	conflict	UNP P08291
g	?	-	SER	deletion	UNP P08291
g	?	-	GLU	deletion	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
g	?	-	SER	deletion	UNP P08291
g	?	-	ILE	deletion	UNP P08291
g	?	-	PRO	deletion	UNP P08291
g	?	-	ALA	deletion	UNP P08291
g	?	-	LEU	deletion	UNP P08291
g	?	-	THR	deletion	UNP P08291
g	?	-	ALA	deletion	UNP P08291
g	?	-	ALA	deletion	UNP P08291
g	?	-	GLU	deletion	UNP P08291
g	?	-	THR	deletion	UNP P08291
g	?	-	GLY	deletion	UNP P08291
g	?	-	HIS	deletion	UNP P08291
g	?	-	THR	deletion	UNP P08291
g	56	ALA	SER	conflict	UNP P08291
g	65	THR	ASN	conflict	UNP P08291
g	86	ARG	LEU	conflict	UNP P08291
g	88	LYS	ARG	conflict	UNP P08291
g	89	LEU	LYS	conflict	UNP P08291
g	90	GLU	LEU	conflict	UNP P08291
g	91	LEU	GLU	conflict	UNP P08291
g	110	GLN	GLU	conflict	UNP P08291
g	124	HIS	GLN	conflict	UNP P08291
g	249	THR	ASN	conflict	UNP P08291
g	258	VAL	SER	conflict	UNP P08291
g	259	GLY	ASN	conflict	UNP P08291
I	21	ARG	LYS	conflict	UNP P08291
I	?	-	SER	deletion	UNP P08291
I	?	-	GLU	deletion	UNP P08291
I	?	-	SER	deletion	UNP P08291
I	?	-	ILE	deletion	UNP P08291
I	?	-	PRO	deletion	UNP P08291
I	?	-	ALA	deletion	UNP P08291
I	?	-	LEU	deletion	UNP P08291
I	?	-	THR	deletion	UNP P08291
I	?	-	ALA	deletion	UNP P08291
I	?	-	ALA	deletion	UNP P08291
I	?	-	GLU	deletion	UNP P08291
I	?	-	THR	deletion	UNP P08291
I	?	-	GLY	deletion	UNP P08291
I	?	-	HIS	deletion	UNP P08291
I	?	-	THR	deletion	UNP P08291
I	56	ALA	SER	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
I	65	THR	ASN	conflict	UNP P08291
I	86	ARG	LEU	conflict	UNP P08291
I	88	LYS	ARG	conflict	UNP P08291
I	89	LEU	LYS	conflict	UNP P08291
I	90	GLU	LEU	conflict	UNP P08291
I	91	LEU	GLU	conflict	UNP P08291
I	110	GLN	GLU	conflict	UNP P08291
I	124	HIS	GLN	conflict	UNP P08291
I	249	THR	ASN	conflict	UNP P08291
I	258	VAL	SER	conflict	UNP P08291
I	259	GLY	ASN	conflict	UNP P08291
M	21	ARG	LYS	conflict	UNP P08291
M	?	-	SER	deletion	UNP P08291
M	?	-	GLU	deletion	UNP P08291
M	?	-	SER	deletion	UNP P08291
M	?	-	ILE	deletion	UNP P08291
M	?	-	PRO	deletion	UNP P08291
M	?	-	ALA	deletion	UNP P08291
M	?	-	LEU	deletion	UNP P08291
M	?	-	THR	deletion	UNP P08291
M	?	-	ALA	deletion	UNP P08291
M	?	-	ALA	deletion	UNP P08291
M	?	-	GLU	deletion	UNP P08291
M	?	-	THR	deletion	UNP P08291
M	?	-	GLY	deletion	UNP P08291
M	?	-	HIS	deletion	UNP P08291
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M	249	THR	ASN	conflict	UNP P08291
M	258	VAL	SER	conflict	UNP P08291
M	259	GLY	ASN	conflict	UNP P08291
Q	21	ARG	LYS	conflict	UNP P08291
Q	?	-	SER	deletion	UNP P08291
Q	?	-	GLU	deletion	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	SER	deletion	UNP P08291
Q	?	-	ILE	deletion	UNP P08291
Q	?	-	PRO	deletion	UNP P08291
Q	?	-	ALA	deletion	UNP P08291
Q	?	-	LEU	deletion	UNP P08291
Q	?	-	THR	deletion	UNP P08291
Q	?	-	ALA	deletion	UNP P08291
Q	?	-	ALA	deletion	UNP P08291
Q	?	-	GLU	deletion	UNP P08291
Q	?	-	THR	deletion	UNP P08291
Q	?	-	GLY	deletion	UNP P08291
Q	?	-	HIS	deletion	UNP P08291
Q	?	-	THR	deletion	UNP P08291
Q	56	ALA	SER	conflict	UNP P08291
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Q	86	ARG	LEU	conflict	UNP P08291
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Q	90	GLU	LEU	conflict	UNP P08291
Q	91	LEU	GLU	conflict	UNP P08291
Q	110	GLN	GLU	conflict	UNP P08291
Q	124	HIS	GLN	conflict	UNP P08291
Q	249	THR	ASN	conflict	UNP P08291
Q	258	VAL	SER	conflict	UNP P08291
Q	259	GLY	ASN	conflict	UNP P08291
U	21	ARG	LYS	conflict	UNP P08291
U	?	-	SER	deletion	UNP P08291
U	?	-	GLU	deletion	UNP P08291
U	?	-	SER	deletion	UNP P08291
U	?	-	ILE	deletion	UNP P08291
U	?	-	PRO	deletion	UNP P08291
U	?	-	ALA	deletion	UNP P08291
U	?	-	LEU	deletion	UNP P08291
U	?	-	THR	deletion	UNP P08291
U	?	-	ALA	deletion	UNP P08291
U	?	-	ALA	deletion	UNP P08291
U	?	-	GLU	deletion	UNP P08291
U	?	-	THR	deletion	UNP P08291
U	?	-	GLY	deletion	UNP P08291
U	?	-	HIS	deletion	UNP P08291
U	?	-	THR	deletion	UNP P08291
U	56	ALA	SER	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
U	65	THR	ASN	conflict	UNP P08291
U	86	ARG	LEU	conflict	UNP P08291
U	88	LYS	ARG	conflict	UNP P08291
U	89	LEU	LYS	conflict	UNP P08291
U	90	GLU	LEU	conflict	UNP P08291
U	91	LEU	GLU	conflict	UNP P08291
U	110	GLN	GLU	conflict	UNP P08291
U	124	HIS	GLN	conflict	UNP P08291
U	249	THR	ASN	conflict	UNP P08291
U	258	VAL	SER	conflict	UNP P08291
U	259	GLY	ASN	conflict	UNP P08291
c	21	ARG	LYS	conflict	UNP P08291
c	?	-	SER	deletion	UNP P08291
c	?	-	GLU	deletion	UNP P08291
c	?	-	SER	deletion	UNP P08291
c	?	-	ILE	deletion	UNP P08291
c	?	-	PRO	deletion	UNP P08291
c	?	-	ALA	deletion	UNP P08291
c	?	-	LEU	deletion	UNP P08291
c	?	-	THR	deletion	UNP P08291
c	?	-	ALA	deletion	UNP P08291
c	?	-	ALA	deletion	UNP P08291
c	?	-	GLU	deletion	UNP P08291
c	?	-	THR	deletion	UNP P08291
c	?	-	GLY	deletion	UNP P08291
c	?	-	HIS	deletion	UNP P08291
c	?	-	THR	deletion	UNP P08291
c	56	ALA	SER	conflict	UNP P08291
c	65	THR	ASN	conflict	UNP P08291
c	86	ARG	LEU	conflict	UNP P08291
c	88	LYS	ARG	conflict	UNP P08291
c	89	LEU	LYS	conflict	UNP P08291
c	90	GLU	LEU	conflict	UNP P08291
c	91	LEU	GLU	conflict	UNP P08291
c	110	GLN	GLU	conflict	UNP P08291
c	124	HIS	GLN	conflict	UNP P08291
c	249	THR	ASN	conflict	UNP P08291
c	258	VAL	SER	conflict	UNP P08291
c	259	GLY	ASN	conflict	UNP P08291
k	21	ARG	LYS	conflict	UNP P08291
k	?	-	SER	deletion	UNP P08291
k	?	-	GLU	deletion	UNP P08291

*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
k	?	-	SER	deletion	UNP P08291
k	?	-	ILE	deletion	UNP P08291
k	?	-	PRO	deletion	UNP P08291
k	?	-	ALA	deletion	UNP P08291
k	?	-	LEU	deletion	UNP P08291
k	?	-	THR	deletion	UNP P08291
k	?	-	ALA	deletion	UNP P08291
k	?	-	ALA	deletion	UNP P08291
k	?	-	GLU	deletion	UNP P08291
k	?	-	THR	deletion	UNP P08291
k	?	-	GLY	deletion	UNP P08291
k	?	-	HIS	deletion	UNP P08291
k	?	-	THR	deletion	UNP P08291
k	56	ALA	SER	conflict	UNP P08291
k	65	THR	ASN	conflict	UNP P08291
k	86	ARG	LEU	conflict	UNP P08291
k	88	LYS	ARG	conflict	UNP P08291
k	89	LEU	LYS	conflict	UNP P08291
k	90	GLU	LEU	conflict	UNP P08291
k	91	LEU	GLU	conflict	UNP P08291
k	110	GLN	GLU	conflict	UNP P08291
k	124	HIS	GLN	conflict	UNP P08291
k	249	THR	ASN	conflict	UNP P08291
k	258	VAL	SER	conflict	UNP P08291
k	259	GLY	ASN	conflict	UNP P08291
o	21	ARG	LYS	conflict	UNP P08291
o	?	-	SER	deletion	UNP P08291
o	?	-	GLU	deletion	UNP P08291
o	?	-	SER	deletion	UNP P08291
o	?	-	ILE	deletion	UNP P08291
o	?	-	PRO	deletion	UNP P08291
o	?	-	ALA	deletion	UNP P08291
o	?	-	LEU	deletion	UNP P08291
o	?	-	THR	deletion	UNP P08291
o	?	-	ALA	deletion	UNP P08291
o	?	-	ALA	deletion	UNP P08291
o	?	-	GLU	deletion	UNP P08291
o	?	-	THR	deletion	UNP P08291
o	?	-	GLY	deletion	UNP P08291
o	?	-	HIS	deletion	UNP P08291
o	?	-	THR	deletion	UNP P08291
o	56	ALA	SER	conflict	UNP P08291

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
o	65	THR	ASN	conflict	UNP P08291
o	86	ARG	LEU	conflict	UNP P08291
o	88	LYS	ARG	conflict	UNP P08291
o	89	LEU	LYS	conflict	UNP P08291
o	90	GLU	LEU	conflict	UNP P08291
o	91	LEU	GLU	conflict	UNP P08291
o	110	GLN	GLU	conflict	UNP P08291
o	124	HIS	GLN	conflict	UNP P08291
o	249	THR	ASN	conflict	UNP P08291
o	258	VAL	SER	conflict	UNP P08291
o	259	GLY	ASN	conflict	UNP P08291
s	21	ARG	LYS	conflict	UNP P08291
s	?	-	SER	deletion	UNP P08291
s	?	-	GLU	deletion	UNP P08291
s	?	-	SER	deletion	UNP P08291
s	?	-	ILE	deletion	UNP P08291
s	?	-	PRO	deletion	UNP P08291
s	?	-	ALA	deletion	UNP P08291
s	?	-	LEU	deletion	UNP P08291
s	?	-	THR	deletion	UNP P08291
s	?	-	ALA	deletion	UNP P08291
s	?	-	ALA	deletion	UNP P08291
s	?	-	GLU	deletion	UNP P08291
s	?	-	THR	deletion	UNP P08291
s	?	-	GLY	deletion	UNP P08291
s	?	-	HIS	deletion	UNP P08291
s	?	-	THR	deletion	UNP P08291
s	56	ALA	SER	conflict	UNP P08291
s	65	THR	ASN	conflict	UNP P08291
s	86	ARG	LEU	conflict	UNP P08291
s	88	LYS	ARG	conflict	UNP P08291
s	89	LEU	LYS	conflict	UNP P08291
s	90	GLU	LEU	conflict	UNP P08291
s	91	LEU	GLU	conflict	UNP P08291
s	110	GLN	GLU	conflict	UNP P08291
s	124	HIS	GLN	conflict	UNP P08291
s	249	THR	ASN	conflict	UNP P08291
s	258	VAL	SER	conflict	UNP P08291
s	259	GLY	ASN	conflict	UNP P08291
w	21	ARG	LYS	conflict	UNP P08291
w	?	-	SER	deletion	UNP P08291
w	?	-	GLU	deletion	UNP P08291

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
w	?	-	SER	deletion	UNP P08291
w	?	-	ILE	deletion	UNP P08291
w	?	-	PRO	deletion	UNP P08291
w	?	-	ALA	deletion	UNP P08291
w	?	-	LEU	deletion	UNP P08291
w	?	-	THR	deletion	UNP P08291
w	?	-	ALA	deletion	UNP P08291
w	?	-	ALA	deletion	UNP P08291
w	?	-	GLU	deletion	UNP P08291
w	?	-	THR	deletion	UNP P08291
w	?	-	GLY	deletion	UNP P08291
w	?	-	HIS	deletion	UNP P08291
w	?	-	THR	deletion	UNP P08291
w	56	ALA	SER	conflict	UNP P08291
w	65	THR	ASN	conflict	UNP P08291
w	86	ARG	LEU	conflict	UNP P08291
w	88	LYS	ARG	conflict	UNP P08291
w	89	LEU	LYS	conflict	UNP P08291
w	90	GLU	LEU	conflict	UNP P08291
w	91	LEU	GLU	conflict	UNP P08291
w	110	GLN	GLU	conflict	UNP P08291
w	124	HIS	GLN	conflict	UNP P08291
w	249	THR	ASN	conflict	UNP P08291
w	258	VAL	SER	conflict	UNP P08291
w	259	GLY	ASN	conflict	UNP P08291
0	21	ARG	LYS	conflict	UNP P08291
0	?	-	SER	deletion	UNP P08291
0	?	-	GLU	deletion	UNP P08291
0	?	-	SER	deletion	UNP P08291
0	?	-	ILE	deletion	UNP P08291
0	?	-	PRO	deletion	UNP P08291
0	?	-	ALA	deletion	UNP P08291
0	?	-	LEU	deletion	UNP P08291
0	?	-	THR	deletion	UNP P08291
0	?	-	ALA	deletion	UNP P08291
0	?	-	ALA	deletion	UNP P08291
0	?	-	GLU	deletion	UNP P08291
0	?	-	THR	deletion	UNP P08291
0	?	-	GLY	deletion	UNP P08291
0	?	-	HIS	deletion	UNP P08291
0	?	-	THR	deletion	UNP P08291
0	56	ALA	SER	conflict	UNP P08291

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*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
0	65	THR	ASN	conflict	UNP P08291
0	86	ARG	LEU	conflict	UNP P08291
0	88	LYS	ARG	conflict	UNP P08291
0	89	LEU	LYS	conflict	UNP P08291
0	90	GLU	LEU	conflict	UNP P08291
0	91	LEU	GLU	conflict	UNP P08291
0	110	GLN	GLU	conflict	UNP P08291
0	124	HIS	GLN	conflict	UNP P08291
0	249	THR	ASN	conflict	UNP P08291
0	258	VAL	SER	conflict	UNP P08291
0	259	GLY	ASN	conflict	UNP P08291
8	21	ARG	LYS	conflict	UNP P08291
8	?	-	SER	deletion	UNP P08291
8	?	-	GLU	deletion	UNP P08291
8	?	-	SER	deletion	UNP P08291
8	?	-	ILE	deletion	UNP P08291
8	?	-	PRO	deletion	UNP P08291
8	?	-	ALA	deletion	UNP P08291
8	?	-	LEU	deletion	UNP P08291
8	?	-	THR	deletion	UNP P08291
8	?	-	ALA	deletion	UNP P08291
8	?	-	ALA	deletion	UNP P08291
8	?	-	GLU	deletion	UNP P08291
8	?	-	THR	deletion	UNP P08291
8	?	-	GLY	deletion	UNP P08291
8	?	-	HIS	deletion	UNP P08291
8	?	-	THR	deletion	UNP P08291
8	56	ALA	SER	conflict	UNP P08291
8	65	THR	ASN	conflict	UNP P08291
8	86	ARG	LEU	conflict	UNP P08291
8	88	LYS	ARG	conflict	UNP P08291
8	89	LEU	LYS	conflict	UNP P08291
8	90	GLU	LEU	conflict	UNP P08291
8	91	LEU	GLU	conflict	UNP P08291
8	110	GLN	GLU	conflict	UNP P08291
8	124	HIS	GLN	conflict	UNP P08291
8	249	THR	ASN	conflict	UNP P08291
8	258	VAL	SER	conflict	UNP P08291
8	259	GLY	ASN	conflict	UNP P08291
AC	21	ARG	LYS	conflict	UNP P08291
AC	?	-	SER	deletion	UNP P08291
AC	?	-	GLU	deletion	UNP P08291

*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	?	-	SER	deletion	UNP P08291
AC	?	-	ILE	deletion	UNP P08291
AC	?	-	PRO	deletion	UNP P08291
AC	?	-	ALA	deletion	UNP P08291
AC	?	-	LEU	deletion	UNP P08291
AC	?	-	THR	deletion	UNP P08291
AC	?	-	ALA	deletion	UNP P08291
AC	?	-	ALA	deletion	UNP P08291
AC	?	-	GLU	deletion	UNP P08291
AC	?	-	THR	deletion	UNP P08291
AC	?	-	GLY	deletion	UNP P08291
AC	?	-	HIS	deletion	UNP P08291
AC	?	-	THR	deletion	UNP P08291
AC	56	ALA	SER	conflict	UNP P08291
AC	65	THR	ASN	conflict	UNP P08291
AC	86	ARG	LEU	conflict	UNP P08291
AC	88	LYS	ARG	conflict	UNP P08291
AC	89	LEU	LYS	conflict	UNP P08291
AC	90	GLU	LEU	conflict	UNP P08291
AC	91	LEU	GLU	conflict	UNP P08291
AC	110	GLN	GLU	conflict	UNP P08291
AC	124	HIS	GLN	conflict	UNP P08291
AC	249	THR	ASN	conflict	UNP P08291
AC	258	VAL	SER	conflict	UNP P08291
AC	259	GLY	ASN	conflict	UNP P08291
AG	21	ARG	LYS	conflict	UNP P08291
AG	?	-	SER	deletion	UNP P08291
AG	?	-	GLU	deletion	UNP P08291
AG	?	-	SER	deletion	UNP P08291
AG	?	-	ILE	deletion	UNP P08291
AG	?	-	PRO	deletion	UNP P08291
AG	?	-	ALA	deletion	UNP P08291
AG	?	-	LEU	deletion	UNP P08291
AG	?	-	THR	deletion	UNP P08291
AG	?	-	ALA	deletion	UNP P08291
AG	?	-	ALA	deletion	UNP P08291
AG	?	-	GLU	deletion	UNP P08291
AG	?	-	THR	deletion	UNP P08291
AG	?	-	GLY	deletion	UNP P08291
AG	?	-	HIS	deletion	UNP P08291
AG	?	-	THR	deletion	UNP P08291
AG	56	ALA	SER	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
AG	65	THR	ASN	conflict	UNP P08291
AG	86	ARG	LEU	conflict	UNP P08291
AG	88	LYS	ARG	conflict	UNP P08291
AG	89	LEU	LYS	conflict	UNP P08291
AG	90	GLU	LEU	conflict	UNP P08291
AG	91	LEU	GLU	conflict	UNP P08291
AG	110	GLN	GLU	conflict	UNP P08291
AG	124	HIS	GLN	conflict	UNP P08291
AG	249	THR	ASN	conflict	UNP P08291
AG	258	VAL	SER	conflict	UNP P08291
AG	259	GLY	ASN	conflict	UNP P08291
AK	21	ARG	LYS	conflict	UNP P08291
AK	?	-	SER	deletion	UNP P08291
AK	?	-	GLU	deletion	UNP P08291
AK	?	-	SER	deletion	UNP P08291
AK	?	-	ILE	deletion	UNP P08291
AK	?	-	PRO	deletion	UNP P08291
AK	?	-	ALA	deletion	UNP P08291
AK	?	-	LEU	deletion	UNP P08291
AK	?	-	THR	deletion	UNP P08291
AK	?	-	ALA	deletion	UNP P08291
AK	?	-	ALA	deletion	UNP P08291
AK	?	-	GLU	deletion	UNP P08291
AK	?	-	THR	deletion	UNP P08291
AK	?	-	GLY	deletion	UNP P08291
AK	?	-	HIS	deletion	UNP P08291
AK	?	-	THR	deletion	UNP P08291
AK	56	ALA	SER	conflict	UNP P08291
AK	65	THR	ASN	conflict	UNP P08291
AK	86	ARG	LEU	conflict	UNP P08291
AK	88	LYS	ARG	conflict	UNP P08291
AK	89	LEU	LYS	conflict	UNP P08291
AK	90	GLU	LEU	conflict	UNP P08291
AK	91	LEU	GLU	conflict	UNP P08291
AK	110	GLN	GLU	conflict	UNP P08291
AK	124	HIS	GLN	conflict	UNP P08291
AK	249	THR	ASN	conflict	UNP P08291
AK	258	VAL	SER	conflict	UNP P08291
AK	259	GLY	ASN	conflict	UNP P08291
AO	21	ARG	LYS	conflict	UNP P08291
AO	?	-	SER	deletion	UNP P08291
AO	?	-	GLU	deletion	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
AO	?	-	SER	deletion	UNP P08291
AO	?	-	ILE	deletion	UNP P08291
AO	?	-	PRO	deletion	UNP P08291
AO	?	-	ALA	deletion	UNP P08291
AO	?	-	LEU	deletion	UNP P08291
AO	?	-	THR	deletion	UNP P08291
AO	?	-	ALA	deletion	UNP P08291
AO	?	-	ALA	deletion	UNP P08291
AO	?	-	GLU	deletion	UNP P08291
AO	?	-	THR	deletion	UNP P08291
AO	?	-	GLY	deletion	UNP P08291
AO	?	-	HIS	deletion	UNP P08291
AO	?	-	THR	deletion	UNP P08291
AO	56	ALA	SER	conflict	UNP P08291
AO	65	THR	ASN	conflict	UNP P08291
AO	86	ARG	LEU	conflict	UNP P08291
AO	88	LYS	ARG	conflict	UNP P08291
AO	89	LEU	LYS	conflict	UNP P08291
AO	90	GLU	LEU	conflict	UNP P08291
AO	91	LEU	GLU	conflict	UNP P08291
AO	110	GLN	GLU	conflict	UNP P08291
AO	124	HIS	GLN	conflict	UNP P08291
AO	249	THR	ASN	conflict	UNP P08291
AO	258	VAL	SER	conflict	UNP P08291
AO	259	GLY	ASN	conflict	UNP P08291

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	2	249	Total	C	H	N	O	S	0	0	0
			3747	1212	1833	321	363	18			
2	B	251	Total	C	H	N	O	S	0	0	0
			3792	1224	1852	327	371	18			
2	F	249	Total	C	H	N	O	S	0	0	0
			3724	1207	1815	320	364	18			
2	Z	249	Total	C	H	N	O	S	0	0	0
			3756	1214	1835	322	367	18			
2	h	250	Total	C	H	N	O	S	0	0	0
			3762	1217	1838	322	367	18			
2	J	249	Total	C	H	N	O	S	0	0	0
			3731	1205	1818	323	367	18			
2	N	251	Total	C	H	N	O	S	0	0	0
			3784	1223	1849	324	370	18			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	R	249	Total	C	H	N	O	S	0	0	0
			3741	1210	1828	322	363	18			
2	V	250	Total	C	H	N	O	S	0	0	0
			3749	1214	1829	322	366	18			
2	d	249	Total	C	H	N	O	S	0	0	0
			3755	1213	1836	324	364	18			
2	l	231	Total	C	H	N	O	S	0	0	0
			3386	1113	1640	290	325	18			
2	p	231	Total	C	H	N	O	S	0	0	0
			3447	1126	1678	295	330	18			
2	t	230	Total	C	H	N	O	S	0	0	0
			3424	1121	1663	293	329	18			
2	x	234	Total	C	H	N	O	S	0	0	0
			3448	1131	1673	296	330	18			
2	5	242	Total	C	H	N	O	S	0	0	0
			3509	1152	1697	302	340	18			
2	9	226	Total	C	H	N	O	S	0	0	0
			3338	1087	1626	288	319	18			
2	AD	232	Total	C	H	N	O	S	0	0	0
			3353	1102	1617	289	327	18			
2	AH	231	Total	C	H	N	O	S	0	0	0
			3325	1096	1602	285	324	18			
2	AL	237	Total	C	H	N	O	S	0	0	0
			3465	1137	1678	297	335	18			
2	AP	226	Total	C	H	N	O	S	0	0	0
			3218	1063	1553	274	310	18			

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	9	PHE	TYR	conflict	UNP P08291
2	49	ALA	GLY	conflict	UNP P08291
2	142	GLU	LYS	conflict	UNP P08291
2	151	THR	ASN	conflict	UNP P08291
2	159	GLN	GLU	conflict	UNP P08291
2	160	ILE	VAL	conflict	UNP P08291
2	162	GLU	THR	conflict	UNP P08291
2	163	THR	SER	conflict	UNP P08291
2	165	SER	ASP	conflict	UNP P08291
2	187	TYR	PHE	conflict	UNP P08291
2	216	PHE	TYR	conflict	UNP P08291
B	9	PHE	TYR	conflict	UNP P08291
B	49	ALA	GLY	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
B	142	GLU	LYS	conflict	UNP P08291
B	151	THR	ASN	conflict	UNP P08291
B	159	GLN	GLU	conflict	UNP P08291
B	160	ILE	VAL	conflict	UNP P08291
B	162	GLU	THR	conflict	UNP P08291
B	163	THR	SER	conflict	UNP P08291
B	165	SER	ASP	conflict	UNP P08291
B	187	TYR	PHE	conflict	UNP P08291
B	216	PHE	TYR	conflict	UNP P08291
F	9	PHE	TYR	conflict	UNP P08291
F	49	ALA	GLY	conflict	UNP P08291
F	142	GLU	LYS	conflict	UNP P08291
F	151	THR	ASN	conflict	UNP P08291
F	159	GLN	GLU	conflict	UNP P08291
F	160	ILE	VAL	conflict	UNP P08291
F	162	GLU	THR	conflict	UNP P08291
F	163	THR	SER	conflict	UNP P08291
F	165	SER	ASP	conflict	UNP P08291
F	187	TYR	PHE	conflict	UNP P08291
F	216	PHE	TYR	conflict	UNP P08291
Z	9	PHE	TYR	conflict	UNP P08291
Z	49	ALA	GLY	conflict	UNP P08291
Z	142	GLU	LYS	conflict	UNP P08291
Z	151	THR	ASN	conflict	UNP P08291
Z	159	GLN	GLU	conflict	UNP P08291
Z	160	ILE	VAL	conflict	UNP P08291
Z	162	GLU	THR	conflict	UNP P08291
Z	163	THR	SER	conflict	UNP P08291
Z	165	SER	ASP	conflict	UNP P08291
Z	187	TYR	PHE	conflict	UNP P08291
Z	216	PHE	TYR	conflict	UNP P08291
h	9	PHE	TYR	conflict	UNP P08291
h	49	ALA	GLY	conflict	UNP P08291
h	142	GLU	LYS	conflict	UNP P08291
h	151	THR	ASN	conflict	UNP P08291
h	159	GLN	GLU	conflict	UNP P08291
h	160	ILE	VAL	conflict	UNP P08291
h	162	GLU	THR	conflict	UNP P08291
h	163	THR	SER	conflict	UNP P08291
h	165	SER	ASP	conflict	UNP P08291
h	187	TYR	PHE	conflict	UNP P08291
h	216	PHE	TYR	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
J	9	PHE	TYR	conflict	UNP P08291
J	49	ALA	GLY	conflict	UNP P08291
J	142	GLU	LYS	conflict	UNP P08291
J	151	THR	ASN	conflict	UNP P08291
J	159	GLN	GLU	conflict	UNP P08291
J	160	ILE	VAL	conflict	UNP P08291
J	162	GLU	THR	conflict	UNP P08291
J	163	THR	SER	conflict	UNP P08291
J	165	SER	ASP	conflict	UNP P08291
J	187	TYR	PHE	conflict	UNP P08291
J	216	PHE	TYR	conflict	UNP P08291
N	9	PHE	TYR	conflict	UNP P08291
N	49	ALA	GLY	conflict	UNP P08291
N	142	GLU	LYS	conflict	UNP P08291
N	151	THR	ASN	conflict	UNP P08291
N	159	GLN	GLU	conflict	UNP P08291
N	160	ILE	VAL	conflict	UNP P08291
N	162	GLU	THR	conflict	UNP P08291
N	163	THR	SER	conflict	UNP P08291
N	165	SER	ASP	conflict	UNP P08291
N	187	TYR	PHE	conflict	UNP P08291
N	216	PHE	TYR	conflict	UNP P08291
R	9	PHE	TYR	conflict	UNP P08291
R	49	ALA	GLY	conflict	UNP P08291
R	142	GLU	LYS	conflict	UNP P08291
R	151	THR	ASN	conflict	UNP P08291
R	159	GLN	GLU	conflict	UNP P08291
R	160	ILE	VAL	conflict	UNP P08291
R	162	GLU	THR	conflict	UNP P08291
R	163	THR	SER	conflict	UNP P08291
R	165	SER	ASP	conflict	UNP P08291
R	187	TYR	PHE	conflict	UNP P08291
R	216	PHE	TYR	conflict	UNP P08291
V	9	PHE	TYR	conflict	UNP P08291
V	49	ALA	GLY	conflict	UNP P08291
V	142	GLU	LYS	conflict	UNP P08291
V	151	THR	ASN	conflict	UNP P08291
V	159	GLN	GLU	conflict	UNP P08291
V	160	ILE	VAL	conflict	UNP P08291
V	162	GLU	THR	conflict	UNP P08291
V	163	THR	SER	conflict	UNP P08291
V	165	SER	ASP	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
V	187	TYR	PHE	conflict	UNP P08291
V	216	PHE	TYR	conflict	UNP P08291
d	9	PHE	TYR	conflict	UNP P08291
d	49	ALA	GLY	conflict	UNP P08291
d	142	GLU	LYS	conflict	UNP P08291
d	151	THR	ASN	conflict	UNP P08291
d	159	GLN	GLU	conflict	UNP P08291
d	160	ILE	VAL	conflict	UNP P08291
d	162	GLU	THR	conflict	UNP P08291
d	163	THR	SER	conflict	UNP P08291
d	165	SER	ASP	conflict	UNP P08291
d	187	TYR	PHE	conflict	UNP P08291
d	216	PHE	TYR	conflict	UNP P08291
l	9	PHE	TYR	conflict	UNP P08291
l	49	ALA	GLY	conflict	UNP P08291
l	142	GLU	LYS	conflict	UNP P08291
l	151	THR	ASN	conflict	UNP P08291
l	159	GLN	GLU	conflict	UNP P08291
l	160	ILE	VAL	conflict	UNP P08291
l	162	GLU	THR	conflict	UNP P08291
l	163	THR	SER	conflict	UNP P08291
l	165	SER	ASP	conflict	UNP P08291
l	187	TYR	PHE	conflict	UNP P08291
l	216	PHE	TYR	conflict	UNP P08291
p	9	PHE	TYR	conflict	UNP P08291
p	49	ALA	GLY	conflict	UNP P08291
p	142	GLU	LYS	conflict	UNP P08291
p	151	THR	ASN	conflict	UNP P08291
p	159	GLN	GLU	conflict	UNP P08291
p	160	ILE	VAL	conflict	UNP P08291
p	162	GLU	THR	conflict	UNP P08291
p	163	THR	SER	conflict	UNP P08291
p	165	SER	ASP	conflict	UNP P08291
p	187	TYR	PHE	conflict	UNP P08291
p	216	PHE	TYR	conflict	UNP P08291
t	9	PHE	TYR	conflict	UNP P08291
t	49	ALA	GLY	conflict	UNP P08291
t	142	GLU	LYS	conflict	UNP P08291
t	151	THR	ASN	conflict	UNP P08291
t	159	GLN	GLU	conflict	UNP P08291
t	160	ILE	VAL	conflict	UNP P08291
t	162	GLU	THR	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
t	163	THR	SER	conflict	UNP P08291
t	165	SER	ASP	conflict	UNP P08291
t	187	TYR	PHE	conflict	UNP P08291
t	216	PHE	TYR	conflict	UNP P08291
x	9	PHE	TYR	conflict	UNP P08291
x	49	ALA	GLY	conflict	UNP P08291
x	142	GLU	LYS	conflict	UNP P08291
x	151	THR	ASN	conflict	UNP P08291
x	159	GLN	GLU	conflict	UNP P08291
x	160	ILE	VAL	conflict	UNP P08291
x	162	GLU	THR	conflict	UNP P08291
x	163	THR	SER	conflict	UNP P08291
x	165	SER	ASP	conflict	UNP P08291
x	187	TYR	PHE	conflict	UNP P08291
x	216	PHE	TYR	conflict	UNP P08291
5	9	PHE	TYR	conflict	UNP P08291
5	49	ALA	GLY	conflict	UNP P08291
5	142	GLU	LYS	conflict	UNP P08291
5	151	THR	ASN	conflict	UNP P08291
5	159	GLN	GLU	conflict	UNP P08291
5	160	ILE	VAL	conflict	UNP P08291
5	162	GLU	THR	conflict	UNP P08291
5	163	THR	SER	conflict	UNP P08291
5	165	SER	ASP	conflict	UNP P08291
5	187	TYR	PHE	conflict	UNP P08291
5	216	PHE	TYR	conflict	UNP P08291
9	9	PHE	TYR	conflict	UNP P08291
9	49	ALA	GLY	conflict	UNP P08291
9	142	GLU	LYS	conflict	UNP P08291
9	151	THR	ASN	conflict	UNP P08291
9	159	GLN	GLU	conflict	UNP P08291
9	160	ILE	VAL	conflict	UNP P08291
9	162	GLU	THR	conflict	UNP P08291
9	163	THR	SER	conflict	UNP P08291
9	165	SER	ASP	conflict	UNP P08291
9	187	TYR	PHE	conflict	UNP P08291
9	216	PHE	TYR	conflict	UNP P08291
AD	9	PHE	TYR	conflict	UNP P08291
AD	49	ALA	GLY	conflict	UNP P08291
AD	142	GLU	LYS	conflict	UNP P08291
AD	151	THR	ASN	conflict	UNP P08291
AD	159	GLN	GLU	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
AD	160	ILE	VAL	conflict	UNP P08291
AD	162	GLU	THR	conflict	UNP P08291
AD	163	THR	SER	conflict	UNP P08291
AD	165	SER	ASP	conflict	UNP P08291
AD	187	TYR	PHE	conflict	UNP P08291
AD	216	PHE	TYR	conflict	UNP P08291
AH	9	PHE	TYR	conflict	UNP P08291
AH	49	ALA	GLY	conflict	UNP P08291
AH	142	GLU	LYS	conflict	UNP P08291
AH	151	THR	ASN	conflict	UNP P08291
AH	159	GLN	GLU	conflict	UNP P08291
AH	160	ILE	VAL	conflict	UNP P08291
AH	162	GLU	THR	conflict	UNP P08291
AH	163	THR	SER	conflict	UNP P08291
AH	165	SER	ASP	conflict	UNP P08291
AH	187	TYR	PHE	conflict	UNP P08291
AH	216	PHE	TYR	conflict	UNP P08291
AL	9	PHE	TYR	conflict	UNP P08291
AL	49	ALA	GLY	conflict	UNP P08291
AL	142	GLU	LYS	conflict	UNP P08291
AL	151	THR	ASN	conflict	UNP P08291
AL	159	GLN	GLU	conflict	UNP P08291
AL	160	ILE	VAL	conflict	UNP P08291
AL	162	GLU	THR	conflict	UNP P08291
AL	163	THR	SER	conflict	UNP P08291
AL	165	SER	ASP	conflict	UNP P08291
AL	187	TYR	PHE	conflict	UNP P08291
AL	216	PHE	TYR	conflict	UNP P08291
AP	9	PHE	TYR	conflict	UNP P08291
AP	49	ALA	GLY	conflict	UNP P08291
AP	142	GLU	LYS	conflict	UNP P08291
AP	151	THR	ASN	conflict	UNP P08291
AP	159	GLN	GLU	conflict	UNP P08291
AP	160	ILE	VAL	conflict	UNP P08291
AP	162	GLU	THR	conflict	UNP P08291
AP	163	THR	SER	conflict	UNP P08291
AP	165	SER	ASP	conflict	UNP P08291
AP	187	TYR	PHE	conflict	UNP P08291
AP	216	PHE	TYR	conflict	UNP P08291

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	3	238	Total	C	H	N	O	S	0	0	0
			3584	1165	1753	298	353	15			
3	C	238	Total	C	H	N	O	S	0	0	0
			3584	1165	1753	298	353	15			
3	G	238	Total	C	H	N	O	S	0	0	0
			3557	1160	1736	294	352	15			
3	a	238	Total	C	H	N	O	S	0	0	0
			3582	1165	1753	296	353	15			
3	i	238	Total	C	H	N	O	S	0	0	0
			3574	1163	1747	297	352	15			
3	K	238	Total	C	H	N	O	S	0	0	0
			3534	1155	1721	293	350	15			
3	O	238	Total	C	H	N	O	S	0	0	0
			3586	1165	1756	299	351	15			
3	S	238	Total	C	H	N	O	S	0	0	0
			3559	1160	1738	295	351	15			
3	W	238	Total	C	H	N	O	S	0	0	0
			3541	1156	1726	295	349	15			
3	e	238	Total	C	H	N	O	S	0	0	0
			3574	1163	1747	297	352	15			
3	m	238	Total	C	H	N	O	S	0	0	0
			3430	1135	1662	283	335	15			
3	q	234	Total	C	H	N	O	S	0	0	0
			3389	1110	1648	285	331	15			
3	u	233	Total	C	H	N	O	S	0	0	0
			3411	1112	1666	288	330	15			
3	y	238	Total	C	H	N	O	S	0	0	0
			3454	1133	1676	289	341	15			
3	6	236	Total	C	H	N	O	S	0	0	0
			3379	1111	1638	285	330	15			
3	AA	234	Total	C	H	N	O	S	0	0	0
			3386	1113	1645	283	330	15			
3	AE	234	Total	C	H	N	O	S	0	0	0
			3403	1114	1659	285	330	15			
3	AI	236	Total	C	H	N	O	S	0	0	0
			3419	1120	1661	284	339	15			
3	AM	234	Total	C	H	N	O	S	0	0	0
			3383	1106	1645	285	332	15			
3	AQ	234	Total	C	H	N	O	S	0	0	0
			3309	1096	1597	274	327	15			

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	59	GLU	ASP	conflict	UNP P08291
3	60	ALA	ASN	conflict	UNP P08291
3	64	SER	GLY	conflict	UNP P08291
3	79	GLY	ARG	conflict	UNP P08291
3	80	LYS	ARG	conflict	UNP P08291
3	93	GLY	ASN	conflict	UNP P08291
3	146	LYS	ARG	conflict	UNP P08291
3	190	ILE	VAL	conflict	UNP P08291
3	199	VAL	ILE	conflict	UNP P08291
3	207	SER	THR	conflict	UNP P08291
3	235	THR	ASN	conflict	UNP P08291
C	59	GLU	ASP	conflict	UNP P08291
C	60	ALA	ASN	conflict	UNP P08291
C	64	SER	GLY	conflict	UNP P08291
C	79	GLY	ARG	conflict	UNP P08291
C	80	LYS	ARG	conflict	UNP P08291
C	93	GLY	ASN	conflict	UNP P08291
C	146	LYS	ARG	conflict	UNP P08291
C	190	ILE	VAL	conflict	UNP P08291
C	199	VAL	ILE	conflict	UNP P08291
C	207	SER	THR	conflict	UNP P08291
C	235	THR	ASN	conflict	UNP P08291
G	59	GLU	ASP	conflict	UNP P08291
G	60	ALA	ASN	conflict	UNP P08291
G	64	SER	GLY	conflict	UNP P08291
G	79	GLY	ARG	conflict	UNP P08291
G	80	LYS	ARG	conflict	UNP P08291
G	93	GLY	ASN	conflict	UNP P08291
G	146	LYS	ARG	conflict	UNP P08291
G	190	ILE	VAL	conflict	UNP P08291
G	199	VAL	ILE	conflict	UNP P08291
G	207	SER	THR	conflict	UNP P08291
G	235	THR	ASN	conflict	UNP P08291
a	59	GLU	ASP	conflict	UNP P08291
a	60	ALA	ASN	conflict	UNP P08291
a	64	SER	GLY	conflict	UNP P08291
a	79	GLY	ARG	conflict	UNP P08291
a	80	LYS	ARG	conflict	UNP P08291
a	93	GLY	ASN	conflict	UNP P08291
a	146	LYS	ARG	conflict	UNP P08291
a	190	ILE	VAL	conflict	UNP P08291
a	199	VAL	ILE	conflict	UNP P08291
a	207	SER	THR	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
a	235	THR	ASN	conflict	UNP P08291
i	59	GLU	ASP	conflict	UNP P08291
i	60	ALA	ASN	conflict	UNP P08291
i	64	SER	GLY	conflict	UNP P08291
i	79	GLY	ARG	conflict	UNP P08291
i	80	LYS	ARG	conflict	UNP P08291
i	93	GLY	ASN	conflict	UNP P08291
i	146	LYS	ARG	conflict	UNP P08291
i	190	ILE	VAL	conflict	UNP P08291
i	199	VAL	ILE	conflict	UNP P08291
i	207	SER	THR	conflict	UNP P08291
i	235	THR	ASN	conflict	UNP P08291
K	59	GLU	ASP	conflict	UNP P08291
K	60	ALA	ASN	conflict	UNP P08291
K	64	SER	GLY	conflict	UNP P08291
K	79	GLY	ARG	conflict	UNP P08291
K	80	LYS	ARG	conflict	UNP P08291
K	93	GLY	ASN	conflict	UNP P08291
K	146	LYS	ARG	conflict	UNP P08291
K	190	ILE	VAL	conflict	UNP P08291
K	199	VAL	ILE	conflict	UNP P08291
K	207	SER	THR	conflict	UNP P08291
K	235	THR	ASN	conflict	UNP P08291
O	59	GLU	ASP	conflict	UNP P08291
O	60	ALA	ASN	conflict	UNP P08291
O	64	SER	GLY	conflict	UNP P08291
O	79	GLY	ARG	conflict	UNP P08291
O	80	LYS	ARG	conflict	UNP P08291
O	93	GLY	ASN	conflict	UNP P08291
O	146	LYS	ARG	conflict	UNP P08291
O	190	ILE	VAL	conflict	UNP P08291
O	199	VAL	ILE	conflict	UNP P08291
O	207	SER	THR	conflict	UNP P08291
O	235	THR	ASN	conflict	UNP P08291
S	59	GLU	ASP	conflict	UNP P08291
S	60	ALA	ASN	conflict	UNP P08291
S	64	SER	GLY	conflict	UNP P08291
S	79	GLY	ARG	conflict	UNP P08291
S	80	LYS	ARG	conflict	UNP P08291
S	93	GLY	ASN	conflict	UNP P08291
S	146	LYS	ARG	conflict	UNP P08291
S	190	ILE	VAL	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
S	199	VAL	ILE	conflict	UNP P08291
S	207	SER	THR	conflict	UNP P08291
S	235	THR	ASN	conflict	UNP P08291
W	59	GLU	ASP	conflict	UNP P08291
W	60	ALA	ASN	conflict	UNP P08291
W	64	SER	GLY	conflict	UNP P08291
W	79	GLY	ARG	conflict	UNP P08291
W	80	LYS	ARG	conflict	UNP P08291
W	93	GLY	ASN	conflict	UNP P08291
W	146	LYS	ARG	conflict	UNP P08291
W	190	ILE	VAL	conflict	UNP P08291
W	199	VAL	ILE	conflict	UNP P08291
W	207	SER	THR	conflict	UNP P08291
W	235	THR	ASN	conflict	UNP P08291
e	59	GLU	ASP	conflict	UNP P08291
e	60	ALA	ASN	conflict	UNP P08291
e	64	SER	GLY	conflict	UNP P08291
e	79	GLY	ARG	conflict	UNP P08291
e	80	LYS	ARG	conflict	UNP P08291
e	93	GLY	ASN	conflict	UNP P08291
e	146	LYS	ARG	conflict	UNP P08291
e	190	ILE	VAL	conflict	UNP P08291
e	199	VAL	ILE	conflict	UNP P08291
e	207	SER	THR	conflict	UNP P08291
e	235	THR	ASN	conflict	UNP P08291
m	59	GLU	ASP	conflict	UNP P08291
m	60	ALA	ASN	conflict	UNP P08291
m	64	SER	GLY	conflict	UNP P08291
m	79	GLY	ARG	conflict	UNP P08291
m	80	LYS	ARG	conflict	UNP P08291
m	93	GLY	ASN	conflict	UNP P08291
m	146	LYS	ARG	conflict	UNP P08291
m	190	ILE	VAL	conflict	UNP P08291
m	199	VAL	ILE	conflict	UNP P08291
m	207	SER	THR	conflict	UNP P08291
m	235	THR	ASN	conflict	UNP P08291
q	59	GLU	ASP	conflict	UNP P08291
q	60	ALA	ASN	conflict	UNP P08291
q	64	SER	GLY	conflict	UNP P08291
q	79	GLY	ARG	conflict	UNP P08291
q	80	LYS	ARG	conflict	UNP P08291
q	93	GLY	ASN	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
q	146	LYS	ARG	conflict	UNP P08291
q	190	ILE	VAL	conflict	UNP P08291
q	199	VAL	ILE	conflict	UNP P08291
q	207	SER	THR	conflict	UNP P08291
q	235	THR	ASN	conflict	UNP P08291
u	59	GLU	ASP	conflict	UNP P08291
u	60	ALA	ASN	conflict	UNP P08291
u	64	SER	GLY	conflict	UNP P08291
u	79	GLY	ARG	conflict	UNP P08291
u	80	LYS	ARG	conflict	UNP P08291
u	93	GLY	ASN	conflict	UNP P08291
u	146	LYS	ARG	conflict	UNP P08291
u	190	ILE	VAL	conflict	UNP P08291
u	199	VAL	ILE	conflict	UNP P08291
u	207	SER	THR	conflict	UNP P08291
u	235	THR	ASN	conflict	UNP P08291
y	59	GLU	ASP	conflict	UNP P08291
y	60	ALA	ASN	conflict	UNP P08291
y	64	SER	GLY	conflict	UNP P08291
y	79	GLY	ARG	conflict	UNP P08291
y	80	LYS	ARG	conflict	UNP P08291
y	93	GLY	ASN	conflict	UNP P08291
y	146	LYS	ARG	conflict	UNP P08291
y	190	ILE	VAL	conflict	UNP P08291
y	199	VAL	ILE	conflict	UNP P08291
y	207	SER	THR	conflict	UNP P08291
y	235	THR	ASN	conflict	UNP P08291
6	59	GLU	ASP	conflict	UNP P08291
6	60	ALA	ASN	conflict	UNP P08291
6	64	SER	GLY	conflict	UNP P08291
6	79	GLY	ARG	conflict	UNP P08291
6	80	LYS	ARG	conflict	UNP P08291
6	93	GLY	ASN	conflict	UNP P08291
6	146	LYS	ARG	conflict	UNP P08291
6	190	ILE	VAL	conflict	UNP P08291
6	199	VAL	ILE	conflict	UNP P08291
6	207	SER	THR	conflict	UNP P08291
6	235	THR	ASN	conflict	UNP P08291
AA	59	GLU	ASP	conflict	UNP P08291
AA	60	ALA	ASN	conflict	UNP P08291
AA	64	SER	GLY	conflict	UNP P08291
AA	79	GLY	ARG	conflict	UNP P08291

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	80	LYS	ARG	conflict	UNP P08291
AA	93	GLY	ASN	conflict	UNP P08291
AA	146	LYS	ARG	conflict	UNP P08291
AA	190	ILE	VAL	conflict	UNP P08291
AA	199	VAL	ILE	conflict	UNP P08291
AA	207	SER	THR	conflict	UNP P08291
AA	235	THR	ASN	conflict	UNP P08291
AE	59	GLU	ASP	conflict	UNP P08291
AE	60	ALA	ASN	conflict	UNP P08291
AE	64	SER	GLY	conflict	UNP P08291
AE	79	GLY	ARG	conflict	UNP P08291
AE	80	LYS	ARG	conflict	UNP P08291
AE	93	GLY	ASN	conflict	UNP P08291
AE	146	LYS	ARG	conflict	UNP P08291
AE	190	ILE	VAL	conflict	UNP P08291
AE	199	VAL	ILE	conflict	UNP P08291
AE	207	SER	THR	conflict	UNP P08291
AE	235	THR	ASN	conflict	UNP P08291
AI	59	GLU	ASP	conflict	UNP P08291
AI	60	ALA	ASN	conflict	UNP P08291
AI	64	SER	GLY	conflict	UNP P08291
AI	79	GLY	ARG	conflict	UNP P08291
AI	80	LYS	ARG	conflict	UNP P08291
AI	93	GLY	ASN	conflict	UNP P08291
AI	146	LYS	ARG	conflict	UNP P08291
AI	190	ILE	VAL	conflict	UNP P08291
AI	199	VAL	ILE	conflict	UNP P08291
AI	207	SER	THR	conflict	UNP P08291
AI	235	THR	ASN	conflict	UNP P08291
AM	59	GLU	ASP	conflict	UNP P08291
AM	60	ALA	ASN	conflict	UNP P08291
AM	64	SER	GLY	conflict	UNP P08291
AM	79	GLY	ARG	conflict	UNP P08291
AM	80	LYS	ARG	conflict	UNP P08291
AM	93	GLY	ASN	conflict	UNP P08291
AM	146	LYS	ARG	conflict	UNP P08291
AM	190	ILE	VAL	conflict	UNP P08291
AM	199	VAL	ILE	conflict	UNP P08291
AM	207	SER	THR	conflict	UNP P08291
AM	235	THR	ASN	conflict	UNP P08291
AQ	59	GLU	ASP	conflict	UNP P08291
AQ	60	ALA	ASN	conflict	UNP P08291

*Continued on next page...*



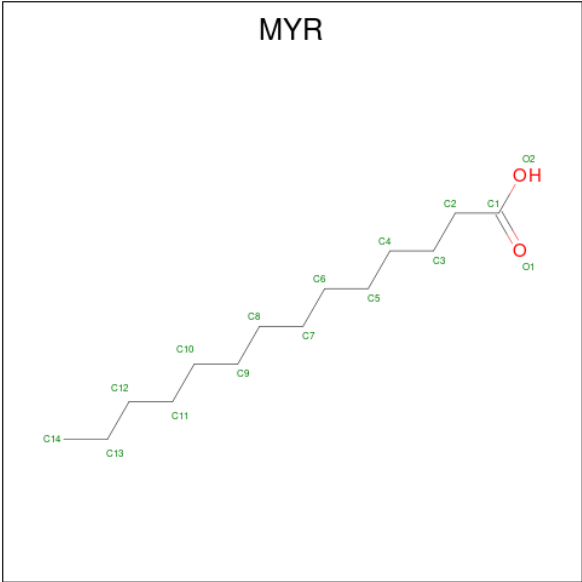
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Chain	Residue	Modelled	Actual	Comment	Reference
AQ	64	SER	GLY	conflict	UNP P08291
AQ	79	GLY	ARG	conflict	UNP P08291
AQ	80	LYS	ARG	conflict	UNP P08291
AQ	93	GLY	ASN	conflict	UNP P08291
AQ	146	LYS	ARG	conflict	UNP P08291
AQ	190	ILE	VAL	conflict	UNP P08291
AQ	199	VAL	ILE	conflict	UNP P08291
AQ	207	SER	THR	conflict	UNP P08291
AQ	235	THR	ASN	conflict	UNP P08291

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	17	Total 242	C 77	H 111	N 25	O 29	0	0	0
4	D	16	Total 243	C 76	H 115	N 25	O 27	0	0	0
4	H	17	Total 258	C 80	H 123	N 26	O 29	0	0	0
4	b	15	Total 226	C 71	H 107	N 23	O 25	0	0	0
4	j	17	Total 258	C 80	H 123	N 26	O 29	0	0	0
4	L	17	Total 240	C 77	H 111	N 23	O 29	0	0	0
4	P	16	Total 243	C 76	H 115	N 25	O 27	0	0	0
4	T	17	Total 258	C 80	H 123	N 26	O 29	0	0	0
4	X	16	Total 240	C 75	H 114	N 24	O 27	0	0	0
4	f	18	Total 270	C 84	H 127	N 27	O 32	0	0	0

- Molecule 5 is MYRISTIC ACID (CCD ID: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

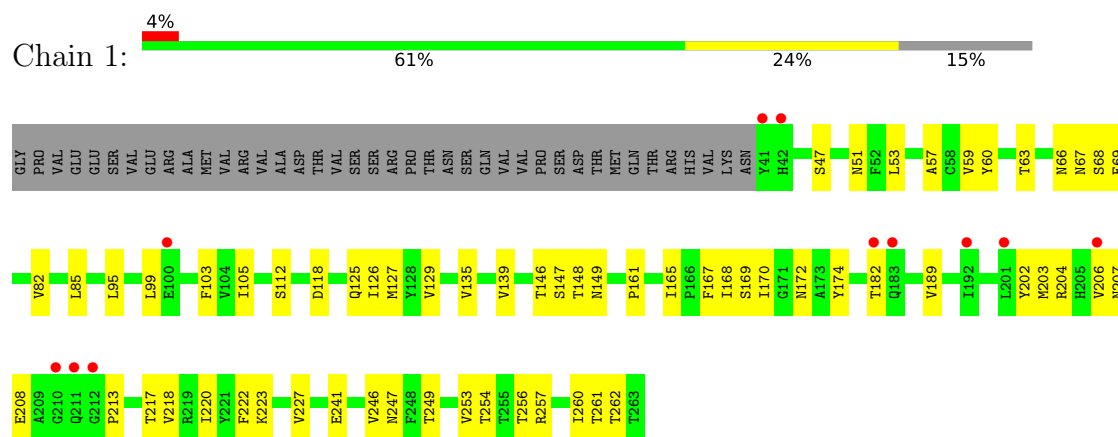


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			43	14	27	2		
5	M	1	Total	C	H	O	0	0
			43	14	27	2		
5	Q	1	Total	C	H	O	0	0
			43	14	27	2		
5	U	1	Total	C	H	O	0	0
			43	14	27	2		

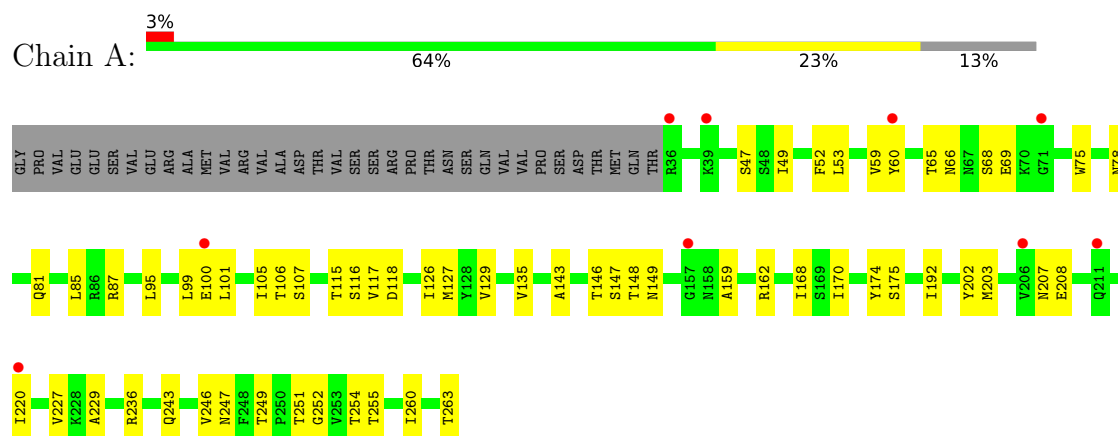
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

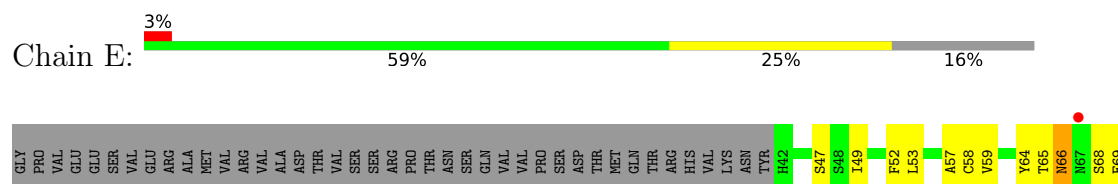
#### • Molecule 1: Capsid protein VP1

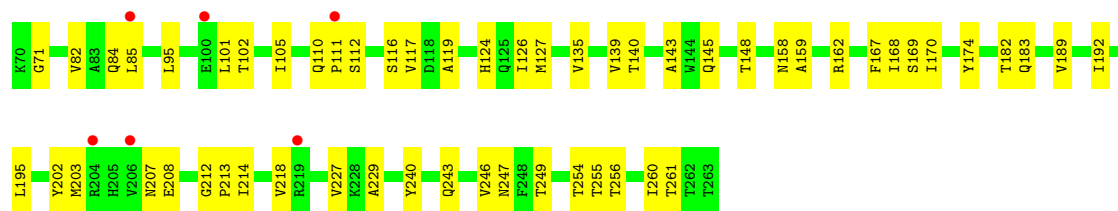


#### • Molecule 1: Capsid protein VP1

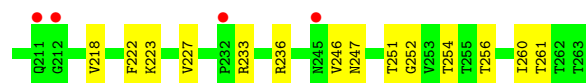
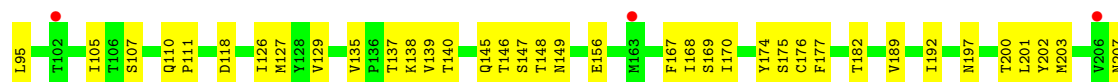
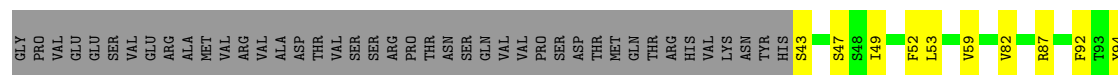


#### • Molecule 1: Capsid protein VP1

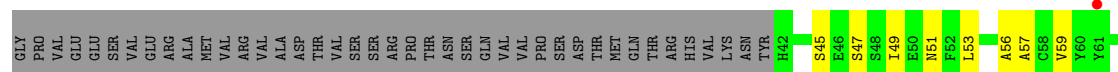




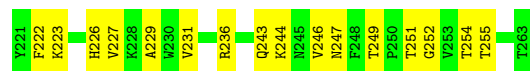
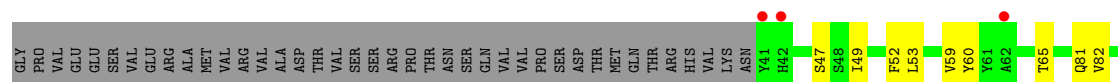
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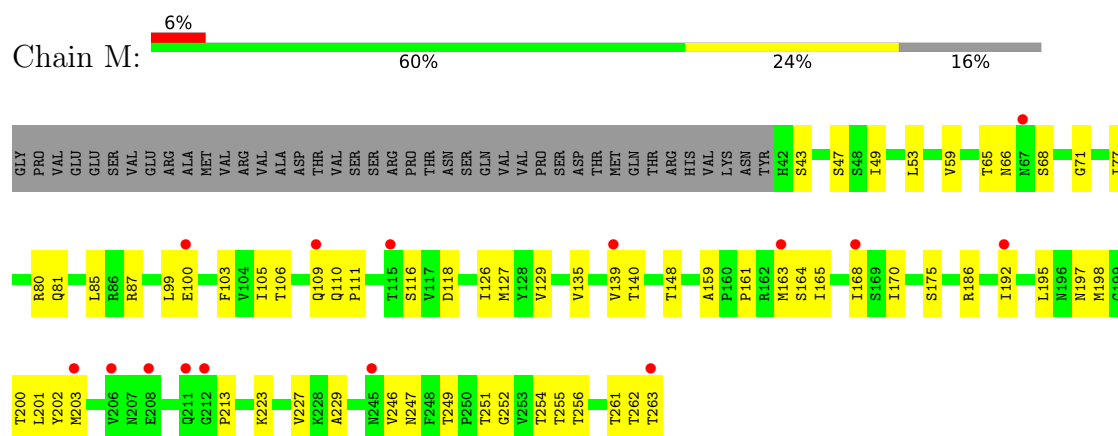
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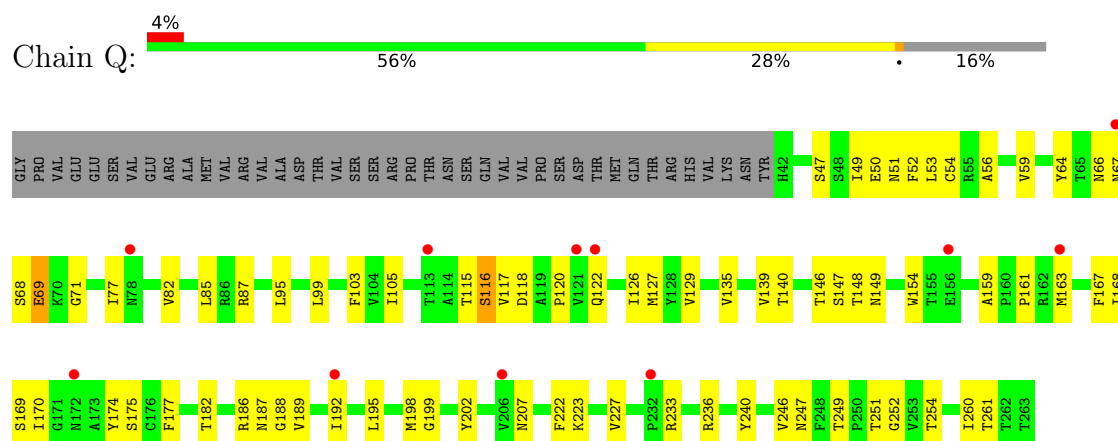
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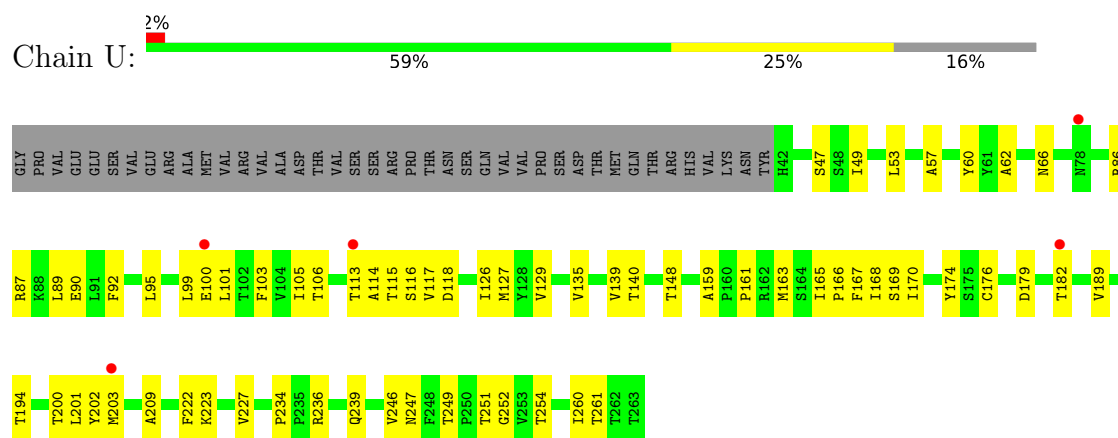
- Molecule 1: Capsid protein VP1



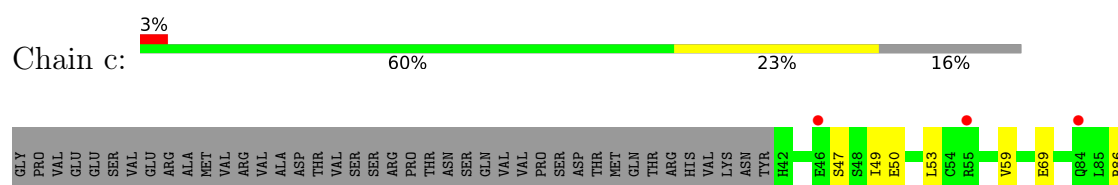
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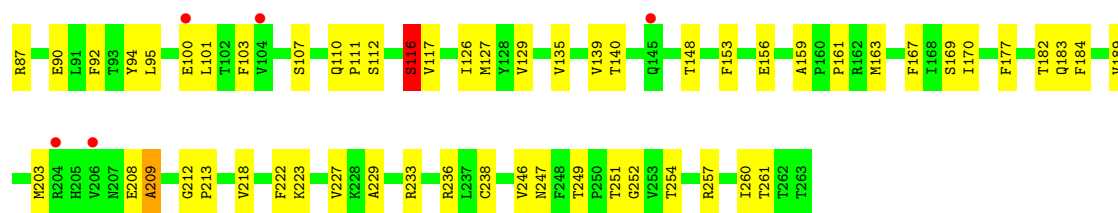


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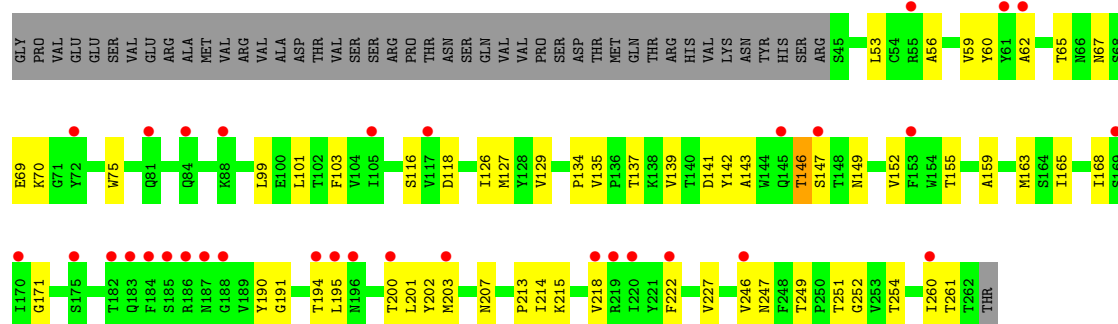


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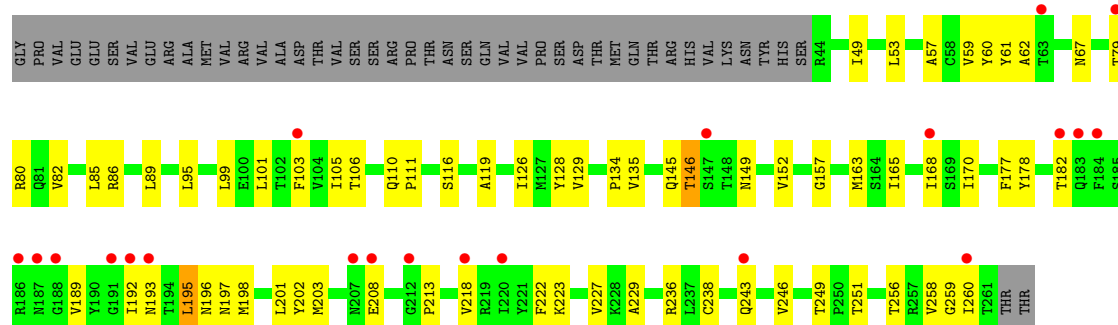




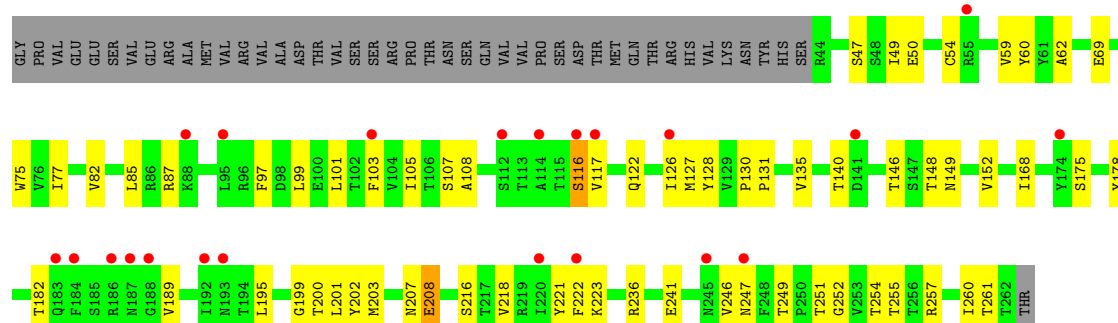
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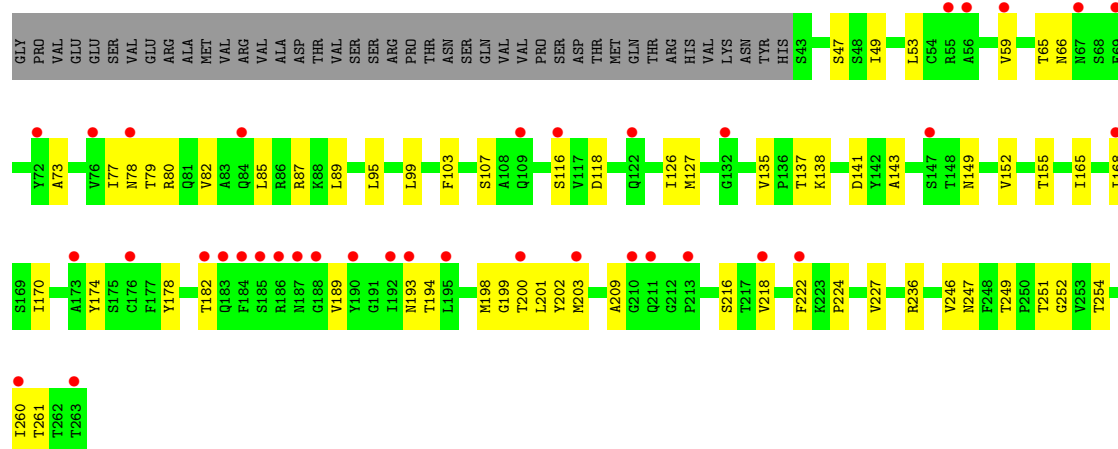
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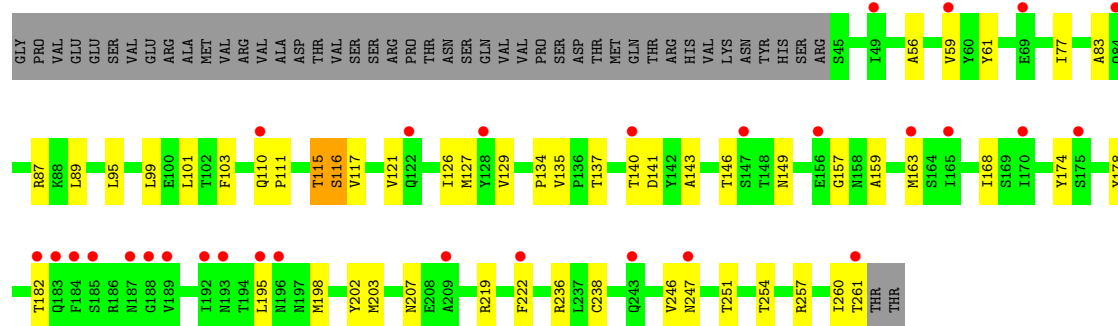
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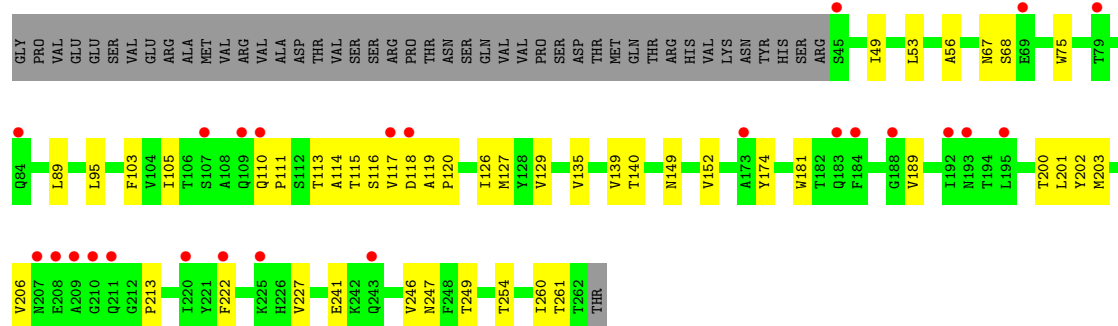
## ● Molecule 1: Capsid protein VP1

Chain w: 

## ● Molecule 1: Capsid protein VP1

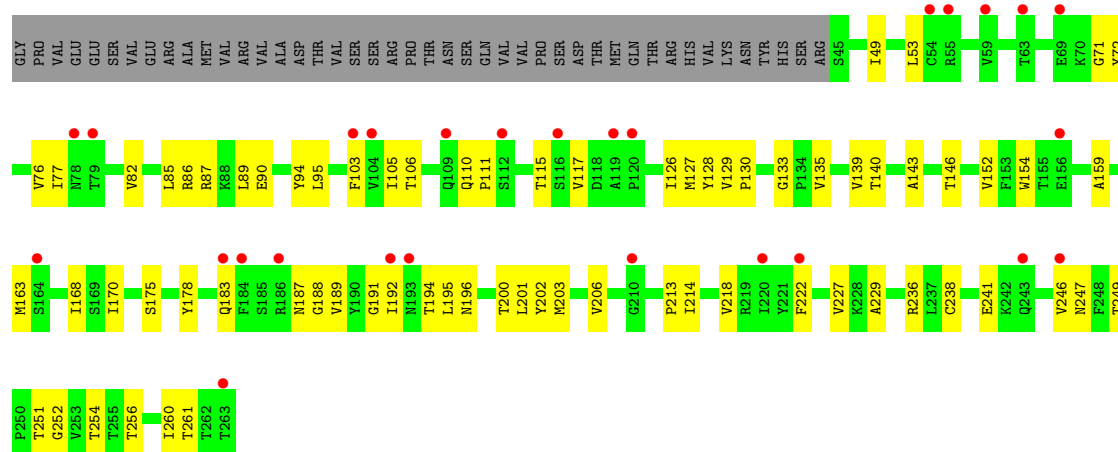
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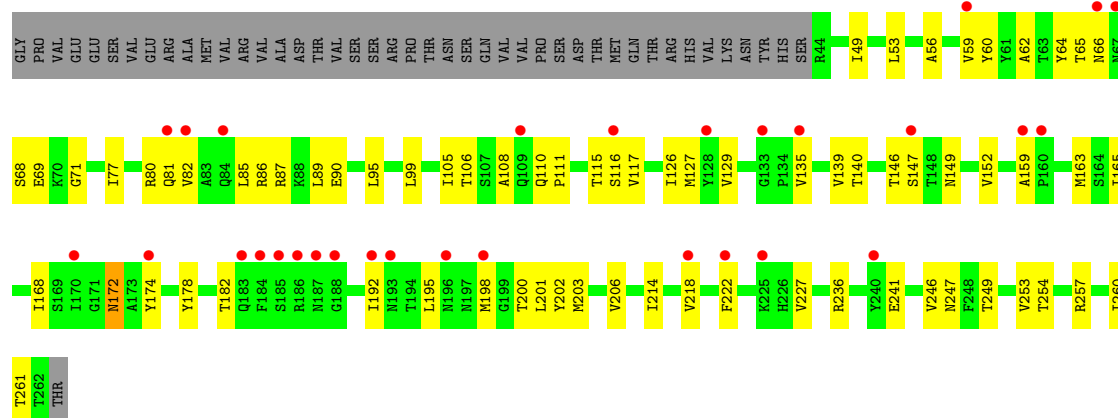
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## ● Molecule 1: Capsid protein VP1

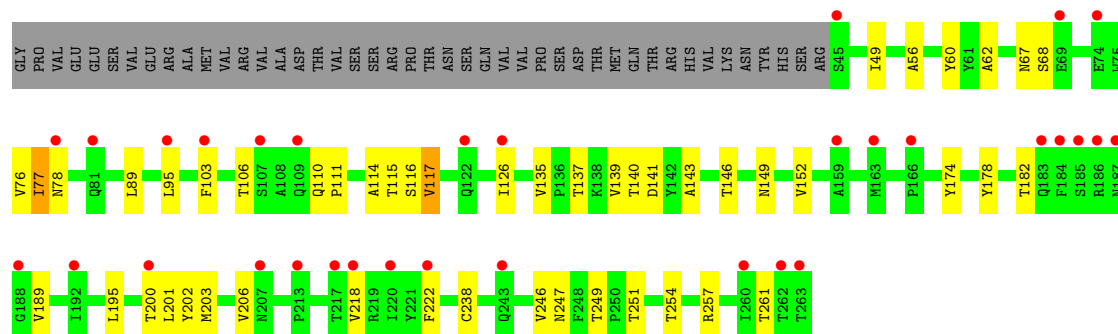
Chain AC: 



• Molecule 1: Capsid protein VP1



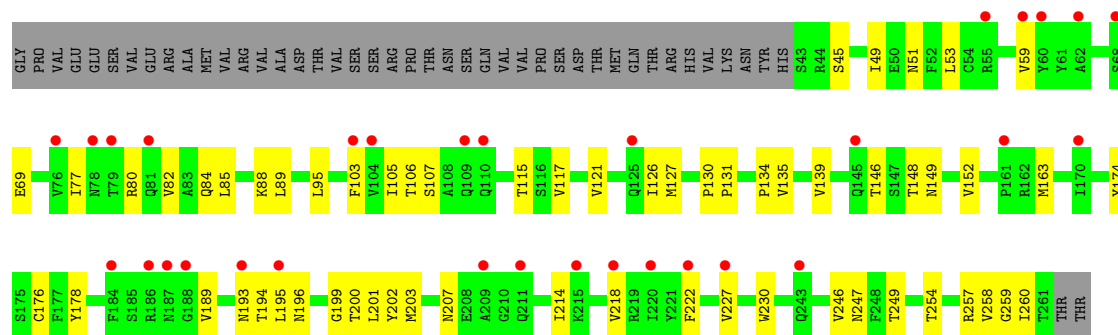
• Molecule 1: Capsid protein VP1



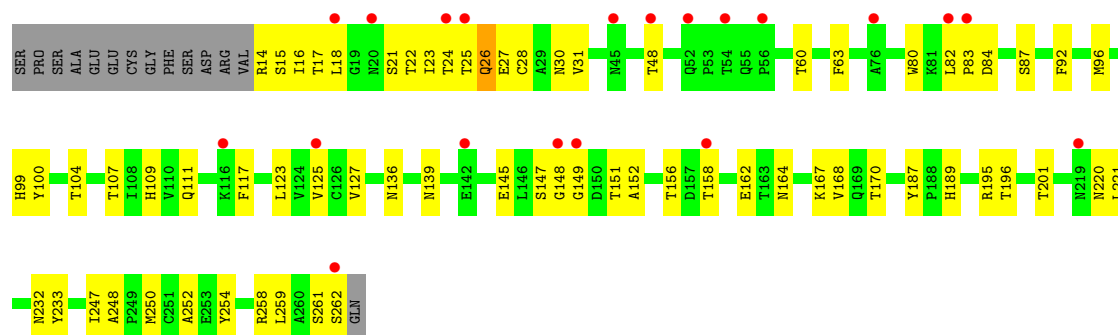
• Molecule 1: Capsid protein VP1



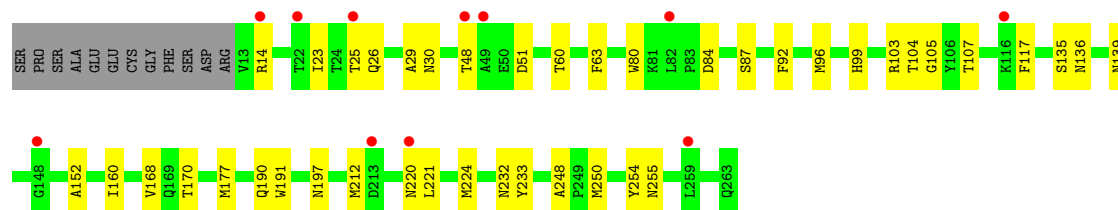
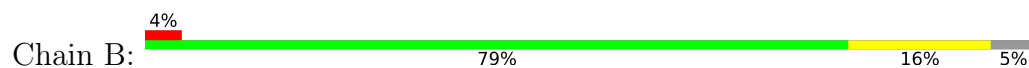




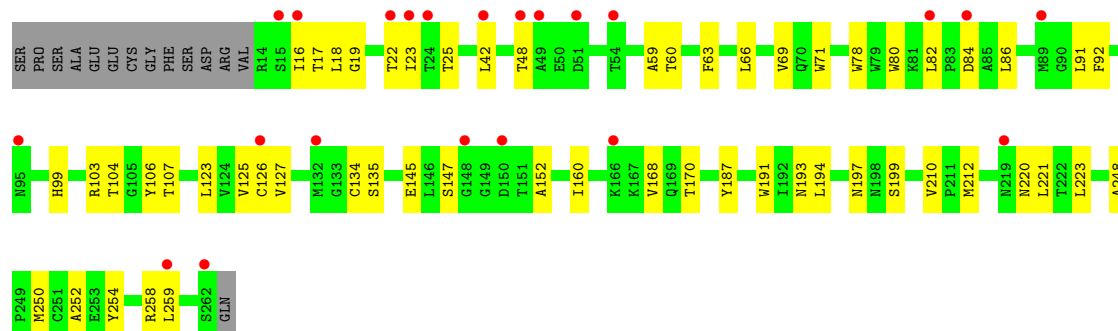
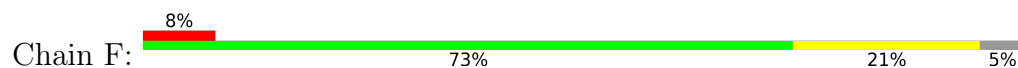
• Molecule 2: Capsid protein VP2



• Molecule 2: Capsid protein VP2

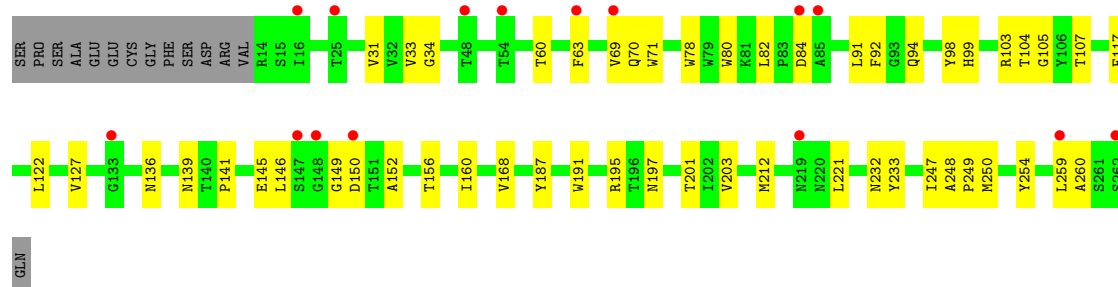


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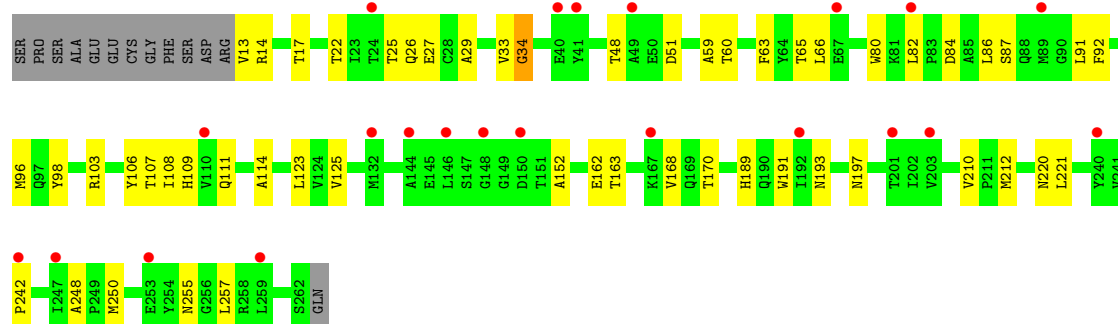
- Molecule 2: Capsid protein VP2

Chain Z: 




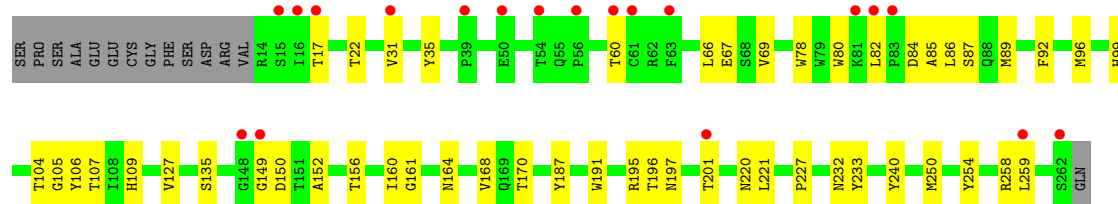
- Molecule 2: Capsid protein VP2

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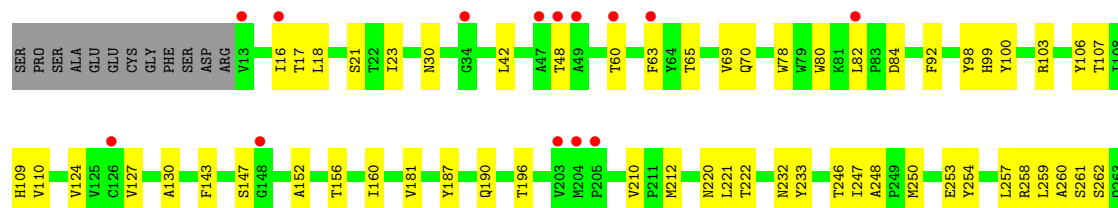
- Molecule 2: Capsid protein VP2

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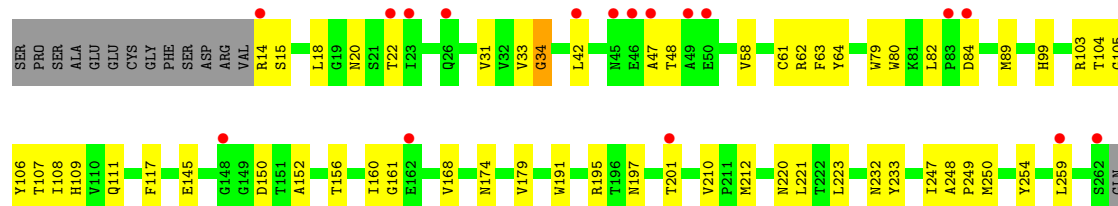
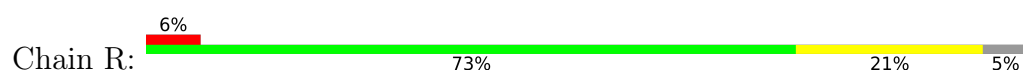


- Molecule 2: Capsid protein VP2

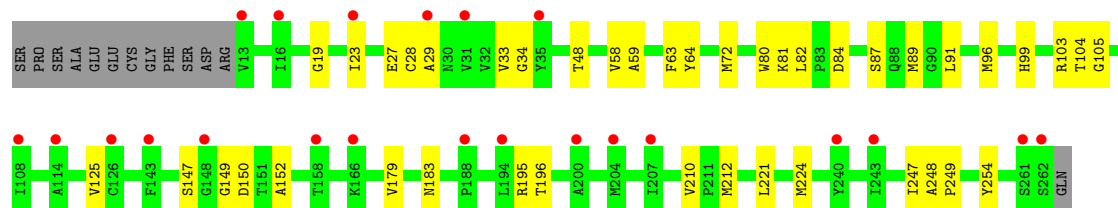
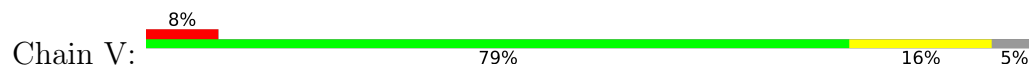
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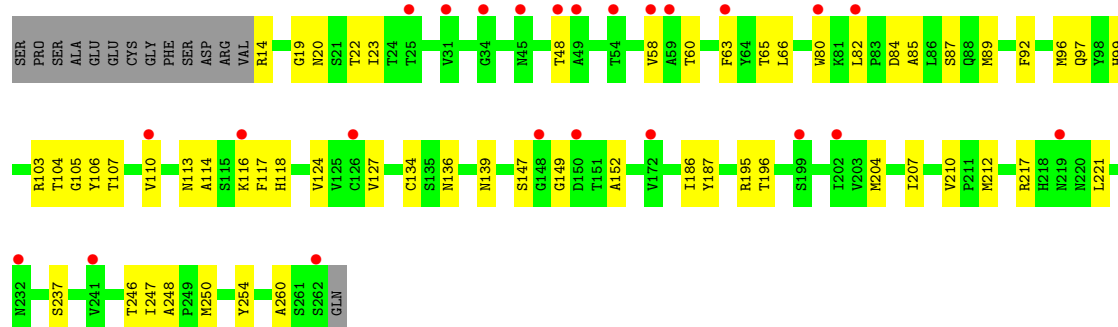
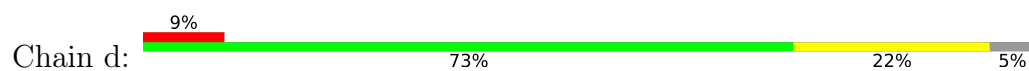
- Molecule 2: Capsid protein VP2



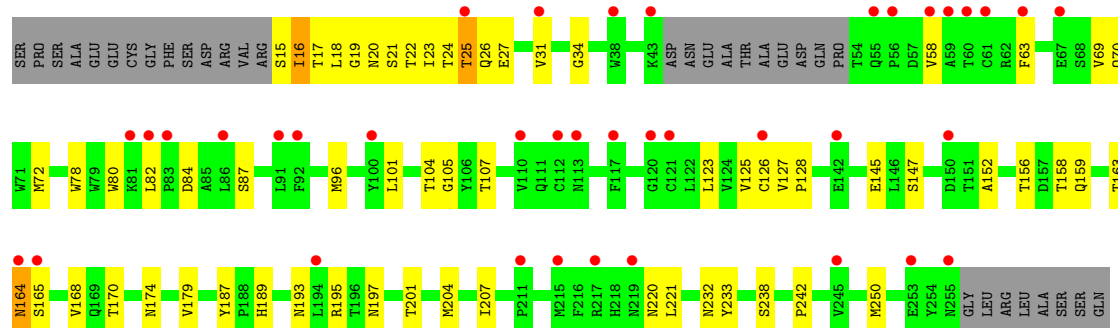
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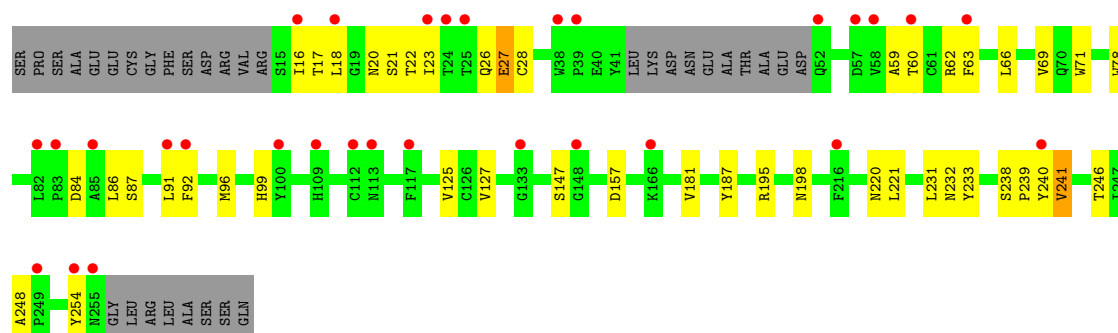
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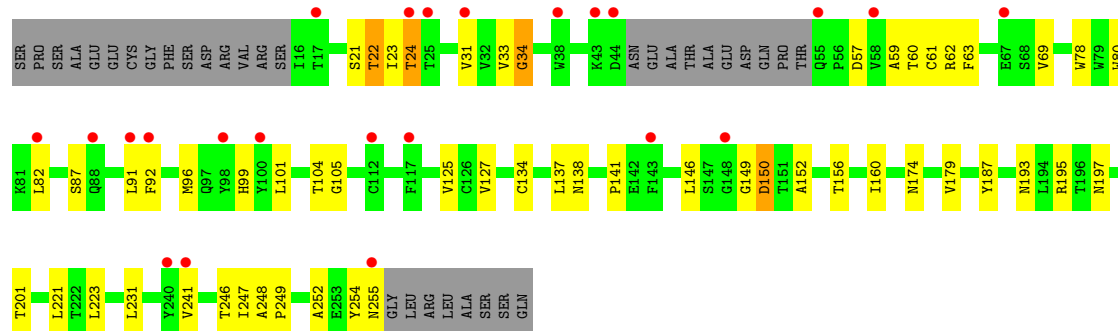
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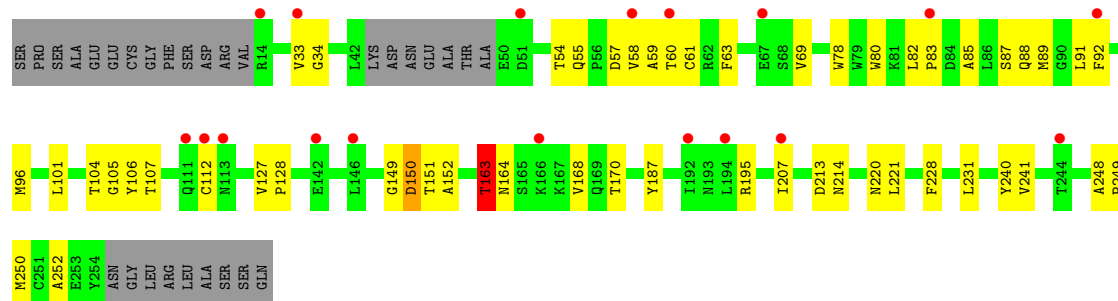
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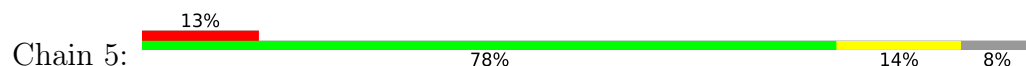
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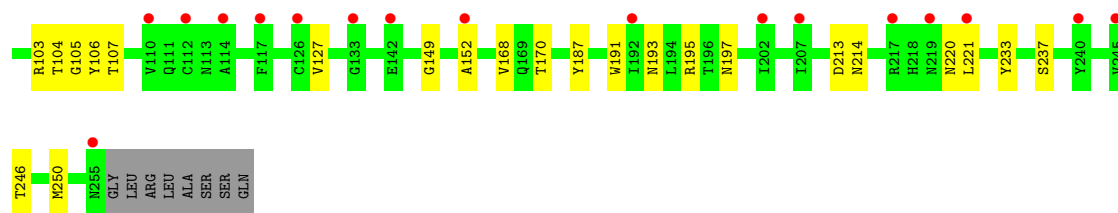


• Molecule 2: Capsid protein VP2



• Molecule 2: Capsid protein VP2

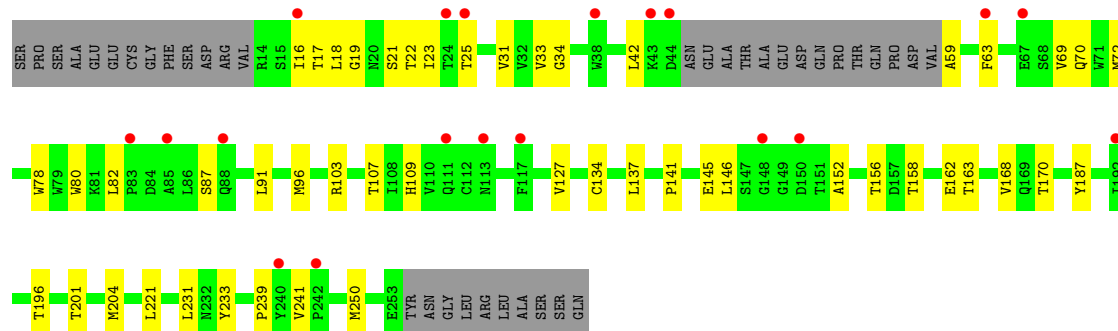




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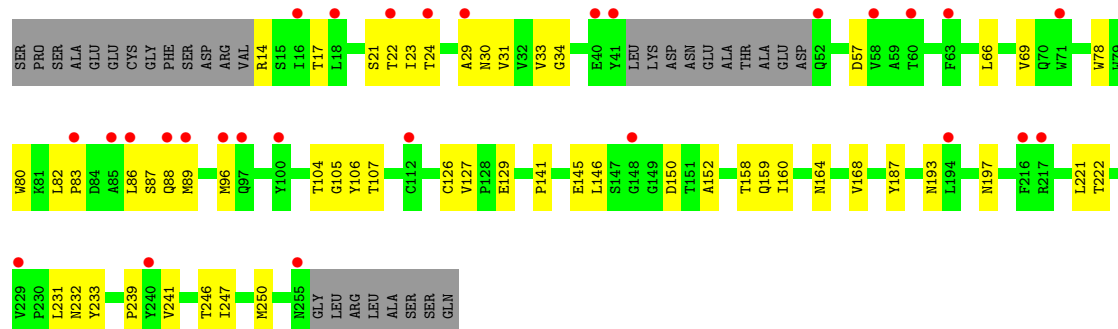
Chain 9:



• Molecule 2: Capsid protein VP2



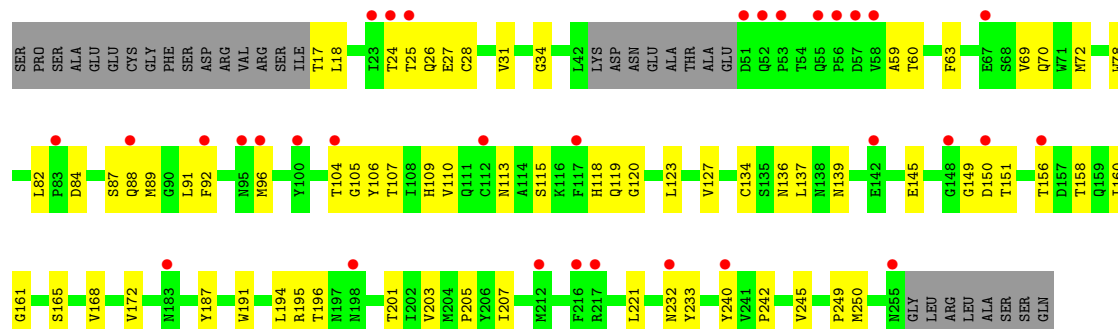
Chain AD:



• Molecule 2: Capsid protein VP2

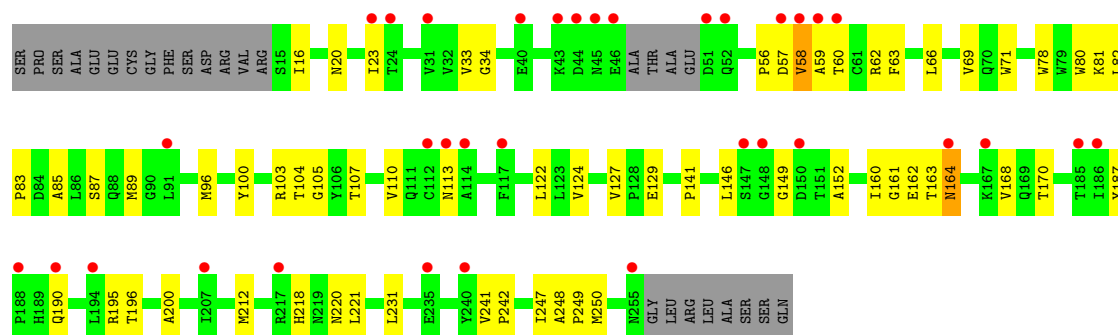


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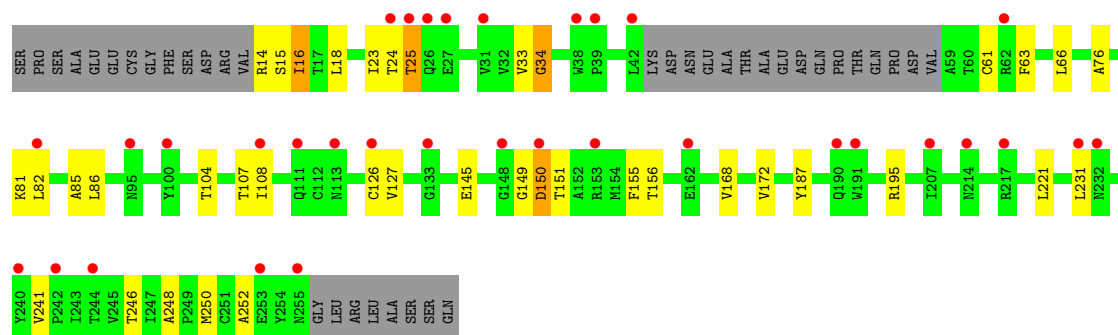
- Molecule 2: Capsid protein VP2

Chain AL: 



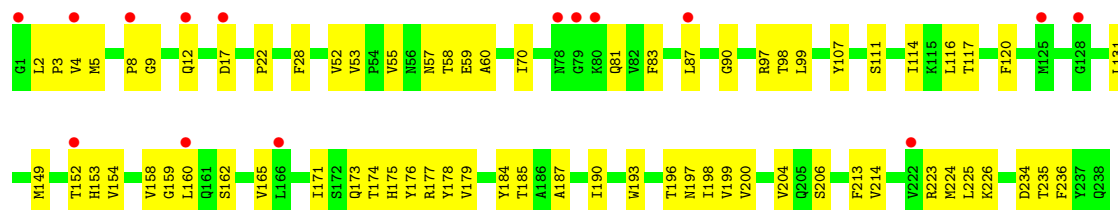
- Molecule 2: Capsid protein VP2

Chain AP: 




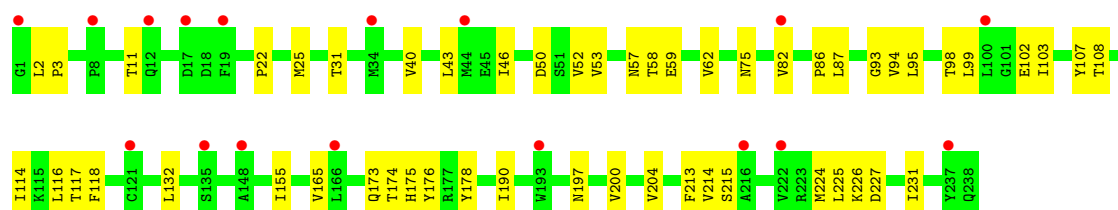
- Molecule 3: Capsid protein VP3

Chain 3: 

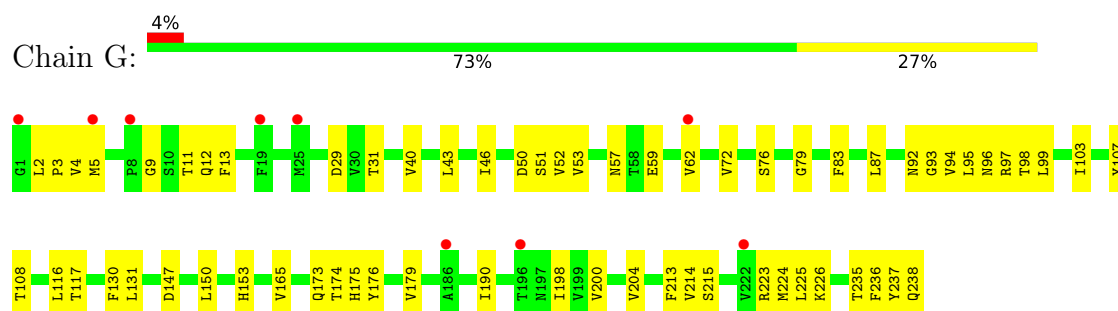


- Molecule 3: Capsid protein VP3

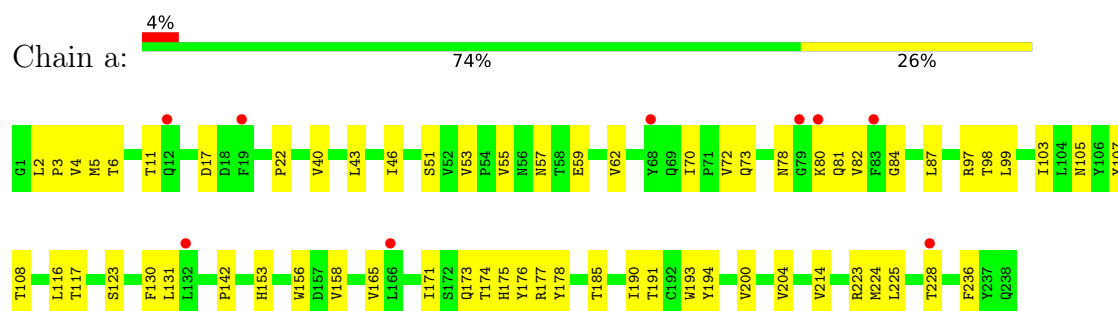
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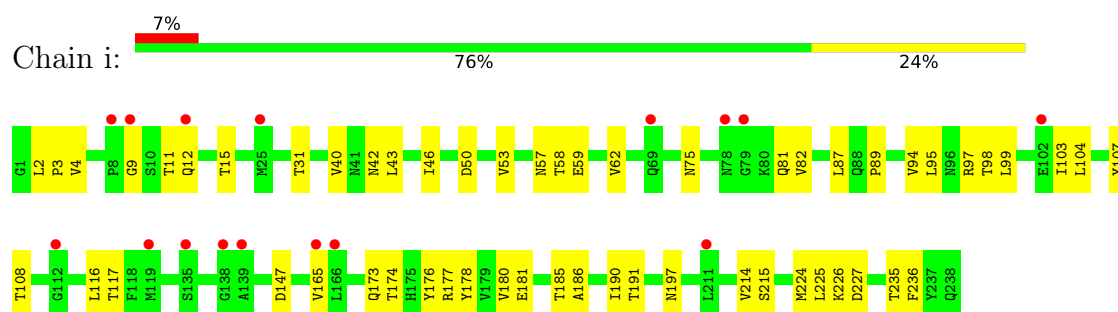
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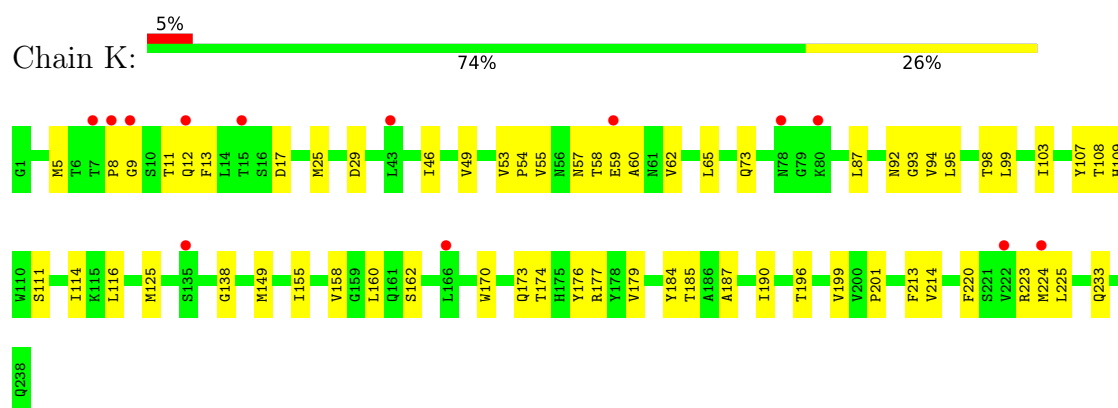
- Molecule 3: Capsid protein VP3



- Molecule 3: Capsid protein VP3

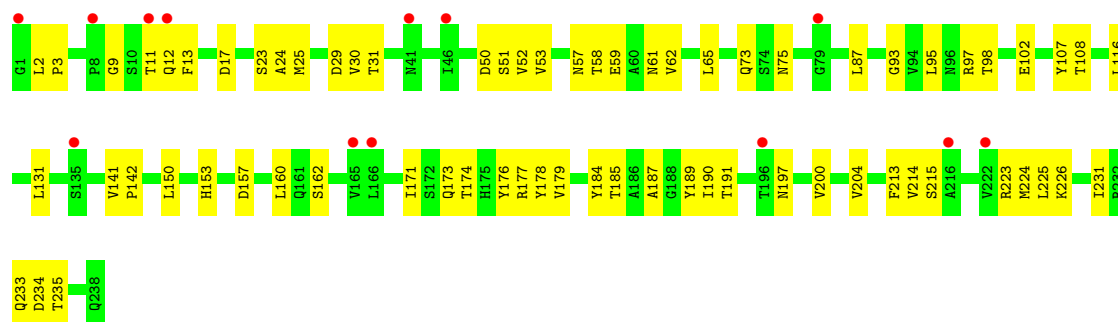


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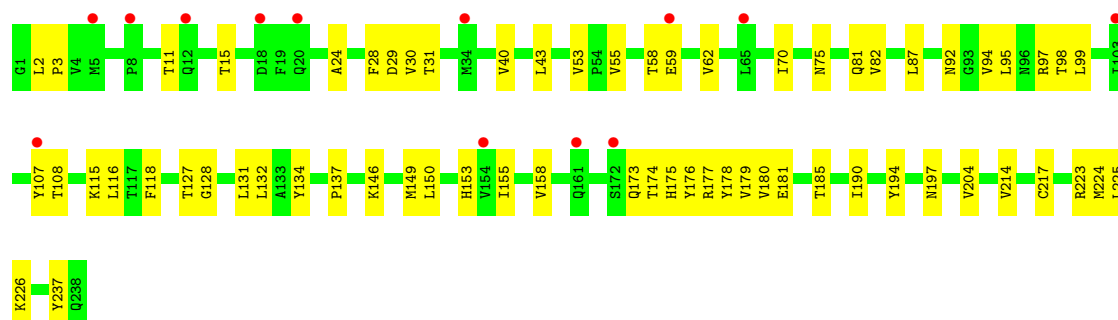
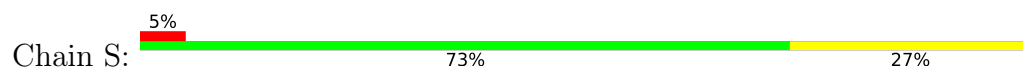


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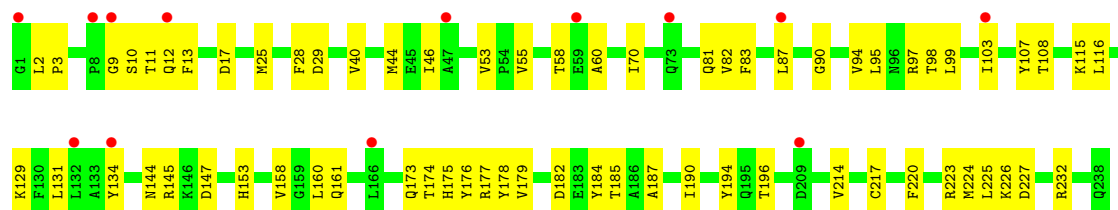
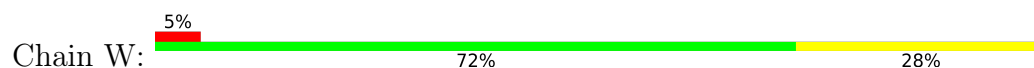




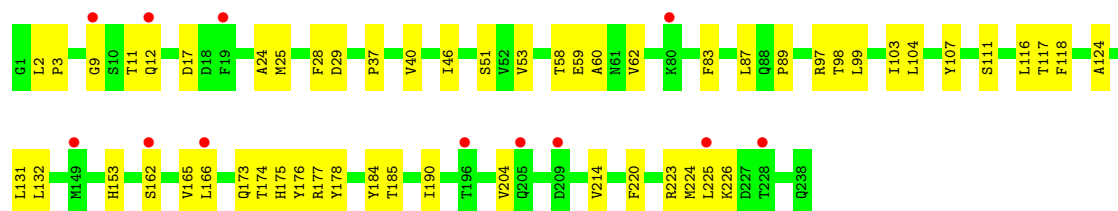
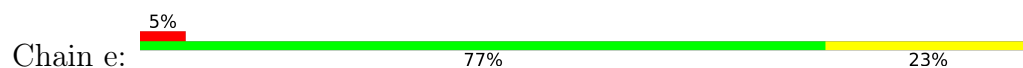
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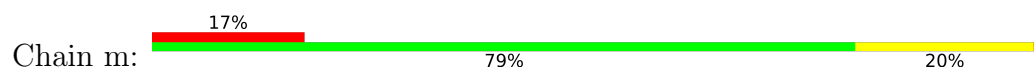
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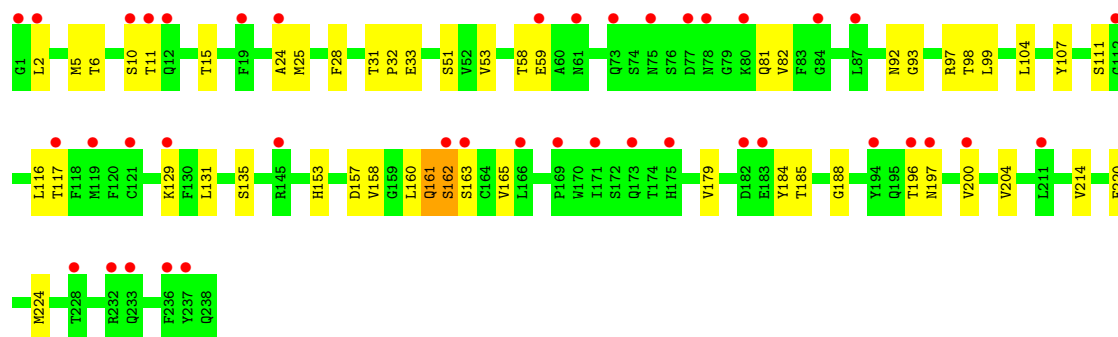
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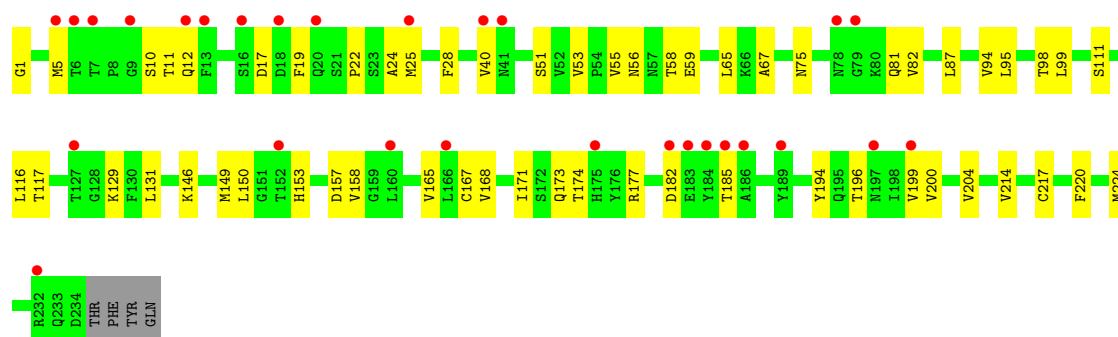
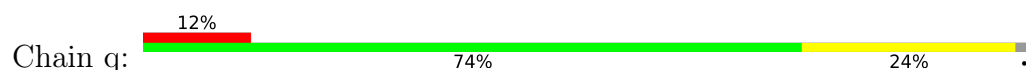
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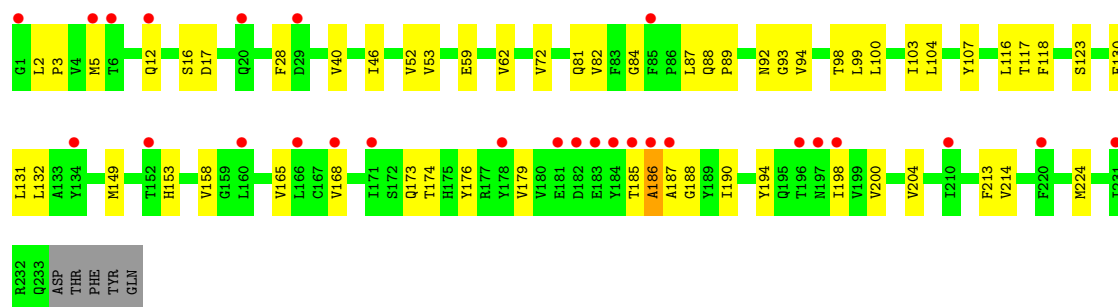
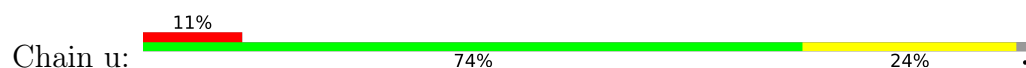




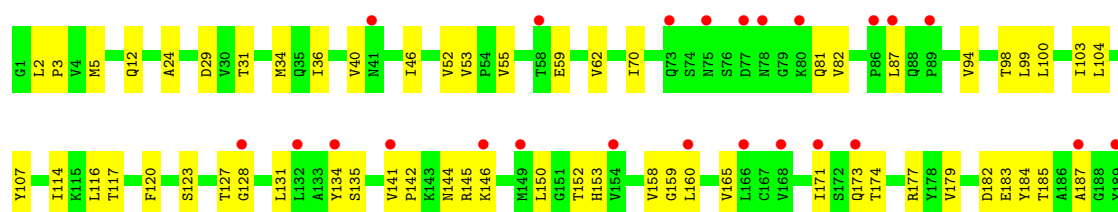
• Molecule 3: Capsid protein VP3



• Molecule 3: Capsid protein VP3

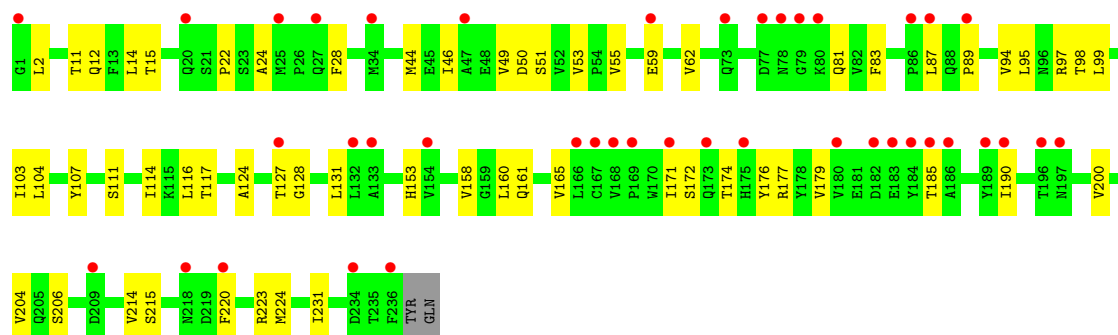
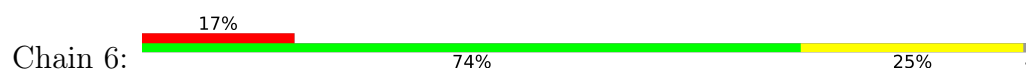


• Molecule 3: Capsid protein VP3

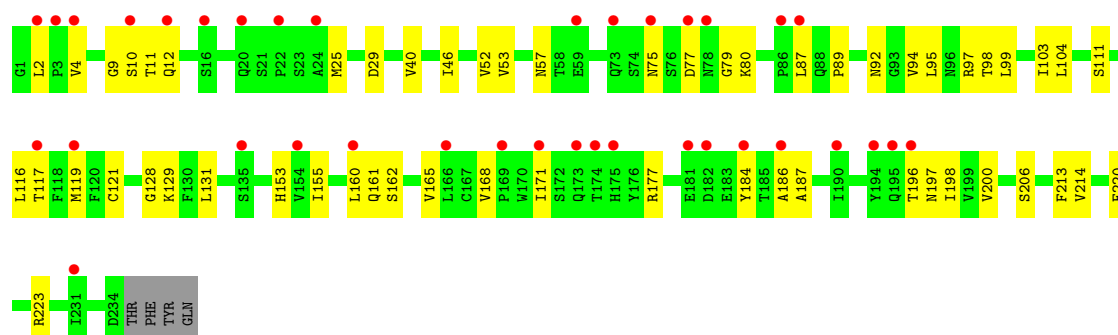
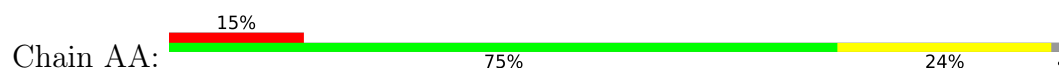




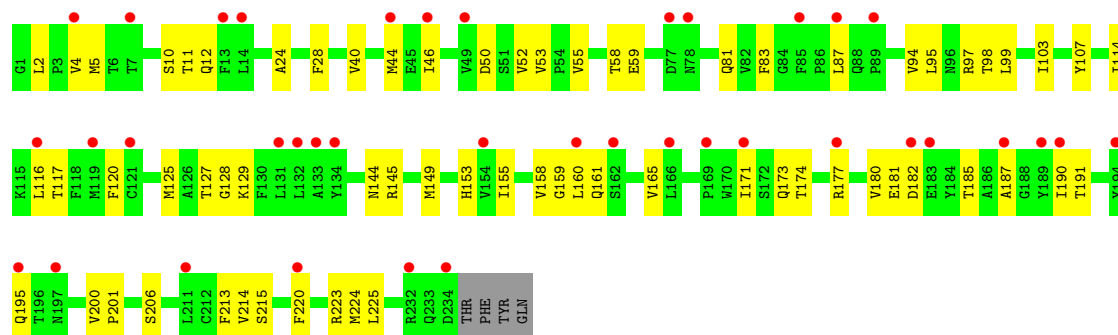
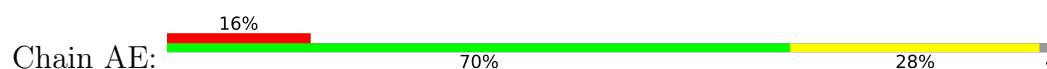
• Molecule 3: Capsid protein VP3



• Molecule 3: Capsid protein VP3

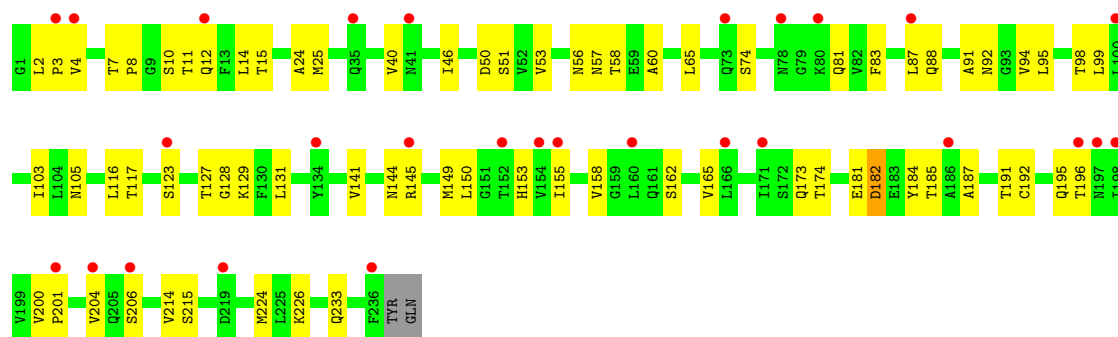


• Molecule 3: Capsid protein VP3

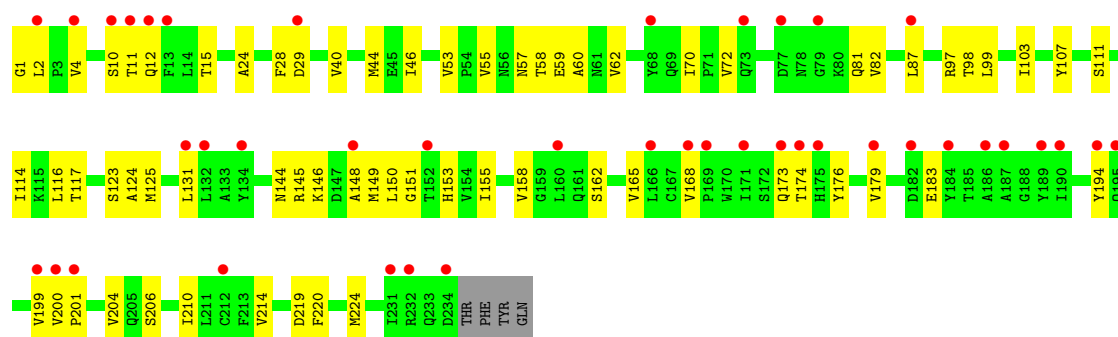


• Molecule 3: Capsid protein VP3

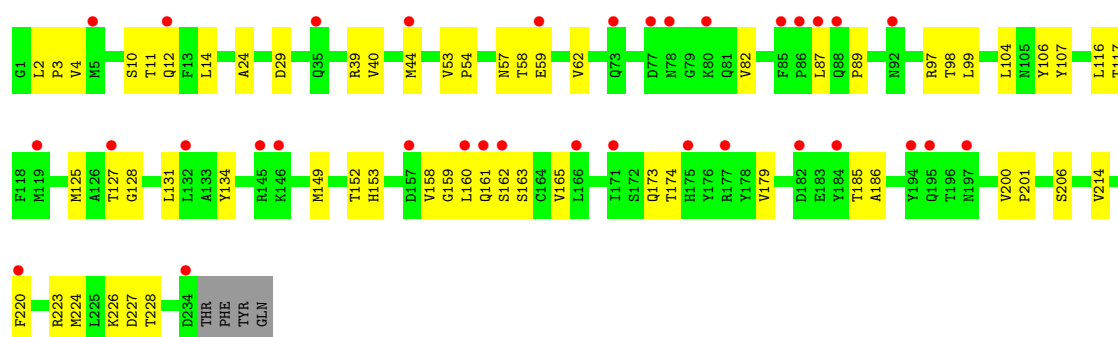
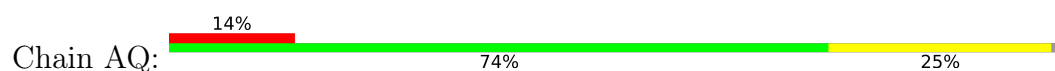




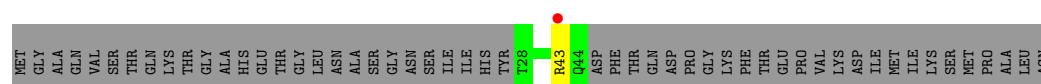
• Molecule 3: Capsid protein VP3



• Molecule 3: Capsid protein VP3

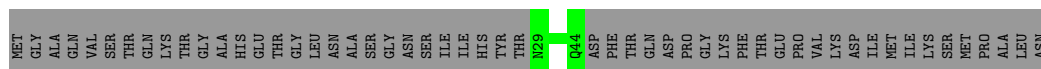


• Molecule 4: Capsid protein VP4

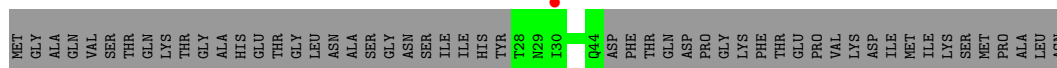


• Molecule 4: Capsid protein VP4

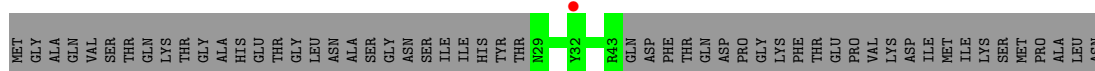




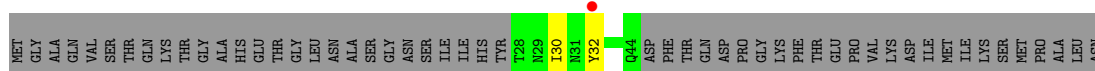
## ● Molecule 4: Capsid protein VP4



## ● Molecule 4: Capsid protein VP4



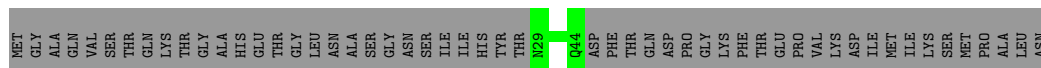
## ● Molecule 4: Capsid protein VP4



## ● Molecule 4: Capsid protein VP4



## ● Molecule 4: Capsid protein VP4



## ● Molecule 4: Capsid protein VP4



## ● Molecule 4: Capsid protein VP4





● Molecule 4: Capsid protein VP4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	344.00Å 344.00Å 457.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.04 – 3.20 97.04 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (97.04-3.20) 99.1 (97.04-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.293 , 0.310 0.293 , 0.309	Depositor DCC
$R_{free}$ test set	25061 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.7	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	211656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYR

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	0.14	0/1739	0.34	0/2384
1	1	0.15	0/1814	0.34	0/2481
1	8	0.15	0/1713	0.35	0/2354
1	A	0.14	0/1864	0.32	0/2552
1	AC	0.16	0/1743	0.36	0/2391
1	AG	0.14	0/1738	0.34	0/2388
1	AK	0.14	0/1738	0.34	0/2386
1	AO	0.14	0/1735	0.35	0/2383
1	E	0.16	0/1819	0.36	0/2488
1	I	0.16	0/1822	0.35	0/2491
1	M	0.16	0/1819	0.37	0/2488
1	Q	0.17	0/1823	0.36	0/2492
1	U	0.16	0/1819	0.34	0/2488
1	Y	0.14	0/1816	0.33	0/2481
1	c	0.14	0/1819	0.33	0/2488
1	g	0.14	0/1823	0.33	0/2492
1	k	0.16	0/1758	0.35	0/2409
1	o	0.14	0/1760	0.34	0/2410
1	s	0.14	0/1762	0.34	0/2414
1	w	0.15	0/1755	0.35	0/2410
2	2	0.15	0/1964	0.39	0/2686
2	5	0.14	0/1861	0.34	0/2555
2	9	0.13	0/1756	0.34	0/2403
2	AD	0.15	0/1783	0.35	0/2448
2	AH	0.14	0/1770	0.35	0/2433
2	AL	0.15	0/1835	0.33	0/2517
2	AP	0.15	0/1709	0.36	0/2345
2	B	0.16	0/1990	0.36	0/2721
2	F	0.15	0/1959	0.35	0/2682
2	J	0.14	0/1962	0.34	0/2686
2	N	0.16	0/1985	0.37	0/2714
2	R	0.16	0/1963	0.36	0/2686

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	V	0.16	0/1970	0.35	0/2697
2	Z	0.14	0/1971	0.33	0/2696
2	d	0.15	0/1969	0.35	0/2693
2	h	0.15	0/1974	0.35	0/2701
2	l	0.14	0/1794	0.36	0/2461
2	p	0.15	0/1818	0.35	0/2491
2	t	0.16	0/1809	0.35	0/2479
2	x	0.18	0/1824	0.37	0/2502
3	3	0.15	0/1879	0.31	0/2570
3	6	0.15	0/1786	0.32	0/2453
3	AA	0.15	0/1787	0.31	0/2453
3	AE	0.15	0/1789	0.33	0/2453
3	AI	0.15	0/1803	0.33	0/2474
3	AM	0.17	0/1782	0.33	0/2445
3	AQ	0.15	0/1757	0.32	0/2416
3	C	0.14	0/1879	0.32	0/2570
3	G	0.16	0/1869	0.35	0/2558
3	K	0.15	0/1861	0.33	0/2549
3	O	0.15	0/1878	0.35	0/2567
3	S	0.15	0/1869	0.33	0/2558
3	W	0.17	0/1863	0.34	0/2551
3	a	0.15	0/1877	0.32	0/2567
3	e	0.14	0/1875	0.32	0/2565
3	i	0.15	0/1875	0.33	0/2565
3	m	0.15	0/1816	0.35	0/2492
3	q	0.16	0/1786	0.35	0/2451
3	u	0.16	0/1790	0.36	0/2454
3	y	0.16	0/1824	0.33	0/2501
4	4	0.08	0/132	0.22	0/179
4	D	0.09	0/129	0.23	0/173
4	H	0.09	0/136	0.24	0/183
4	L	0.11	0/130	0.28	0/176
4	P	0.17	0/129	0.30	0/173
4	T	0.13	0/136	0.26	0/183
4	X	0.13	0/127	0.25	0/171
4	b	0.09	0/120	0.26	0/161
4	f	0.10	0/144	0.21	0/194
4	j	0.10	0/136	0.41	0/183
All	All	0.15	0/111309	0.34	0/152454

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1689	1612	1611	45	0
1	1	1763	1709	1708	58	0
1	8	1664	1566	1565	39	0
1	A	1810	1736	1736	55	0
1	AC	1693	1603	1602	69	0
1	AG	1688	1586	1585	63	0
1	AK	1688	1599	1598	44	0
1	AO	1685	1580	1579	52	0
1	E	1767	1712	1712	57	0
1	I	1771	1722	1720	54	0
1	M	1767	1714	1712	54	0
1	Q	1771	1723	1723	62	0
1	U	1767	1712	1712	61	0
1	Y	1765	1728	1727	53	0
1	c	1767	1713	1712	55	0
1	g	1771	1724	1723	52	0
1	k	1707	1627	1626	59	2
1	o	1710	1649	1648	66	0
1	s	1712	1640	1639	61	0
1	w	1704	1600	1599	56	0
2	2	1914	1833	1832	62	1
2	5	1812	1697	1696	24	0
2	9	1712	1626	1625	44	0
2	AD	1736	1617	1616	41	0
2	AH	1723	1602	1600	57	0
2	AL	1787	1678	1677	43	0
2	AP	1665	1553	1552	36	0
2	B	1940	1852	1852	29	0
2	F	1909	1815	1814	48	0
2	J	1913	1818	1817	38	1
2	N	1935	1849	1848	42	0
2	R	1913	1828	1827	44	0
2	V	1920	1829	1829	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	1921	1835	1835	37	0
2	d	1919	1836	1836	49	0
2	h	1924	1838	1838	46	0
2	l	1746	1640	1638	56	0
2	p	1769	1678	1677	34	0
2	t	1761	1663	1662	41	1
2	x	1775	1673	1671	45	1
3	3	1831	1753	1753	73	0
3	6	1741	1638	1638	55	0
3	AA	1741	1645	1645	48	0
3	AE	1744	1659	1659	60	0
3	AI	1758	1661	1661	63	1
3	AM	1738	1645	1645	57	0
3	AQ	1712	1597	1597	51	0
3	C	1831	1753	1753	51	1
3	G	1821	1736	1736	59	2
3	K	1813	1721	1721	64	0
3	O	1830	1756	1756	64	0
3	S	1821	1738	1738	56	0
3	W	1815	1726	1726	67	0
3	a	1829	1753	1753	58	1
3	e	1827	1747	1747	48	0
3	i	1827	1747	1747	49	0
3	m	1768	1662	1662	49	0
3	q	1741	1648	1648	46	0
3	u	1745	1666	1666	45	1
3	y	1778	1676	1676	62	0
4	4	131	111	111	1	0
4	D	128	115	115	0	0
4	H	135	123	122	0	0
4	L	129	111	111	1	0
4	P	128	115	115	0	0
4	T	135	123	122	3	0
4	X	126	114	114	3	0
4	b	119	107	107	0	0
4	f	143	127	126	1	0
4	j	135	123	122	2	0
5	A	16	27	27	0	0
5	M	16	27	27	2	0
5	Q	16	27	27	2	0
5	U	16	27	27	4	0
All	All	108437	103219	103179	2614	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 2614 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:14:ARG:N	2:AD:24:THR:HG1	1.42	1.16
2:5:107:THR:OG1	2:5:250:MET:SD	2.22	0.97
3:AM:117:THR:HG23	3:AM:165:VAL:HG22	1.46	0.97
2:p:23:ILE:HD11	2:p:246:THR:HG21	1.46	0.96
1:AK:203:MET:HE3	1:AK:218:VAL:HG21	1.43	0.96

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:24:THR:OG1	3:C:155:ILE:O[6_565]	2.00	0.20
2:x:240:TYR:OH	3:AI:74:SER:OG[3_565]	2.07	0.13
3:a:78:ASN:OD1	2:J:240:TYR:OH[4_555]	2.09	0.11
3:G:76:SER:O	1:k:67:ASN:HD22[6_565]	1.55	0.05
3:G:76:SER:O	1:k:67:ASN:ND2[6_565]	2.16	0.04

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	215/263 (82%)	198 (92%)	15 (7%)	2 (1%)	14	47
1	1	221/263 (84%)	201 (91%)	20 (9%)	0	100	100
1	8	216/263 (82%)	193 (89%)	23 (11%)	0	100	100
1	A	226/263 (86%)	213 (94%)	13 (6%)	0	100	100
1	AC	217/263 (82%)	191 (88%)	25 (12%)	1 (0%)	24	59
1	AG	217/263 (82%)	197 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AK	217/263 (82%)	195 (90%)	20 (9%)	2 (1%)	14	47
1	AO	217/263 (82%)	197 (91%)	20 (9%)	0	100	100
1	E	220/263 (84%)	203 (92%)	15 (7%)	2 (1%)	14	47
1	I	221/263 (84%)	206 (93%)	15 (7%)	0	100	100
1	M	220/263 (84%)	204 (93%)	16 (7%)	0	100	100
1	Q	220/263 (84%)	204 (93%)	14 (6%)	2 (1%)	14	47
1	U	220/263 (84%)	200 (91%)	20 (9%)	0	100	100
1	Y	219/263 (83%)	204 (93%)	15 (7%)	0	100	100
1	c	220/263 (84%)	203 (92%)	15 (7%)	2 (1%)	14	47
1	g	220/263 (84%)	205 (93%)	13 (6%)	2 (1%)	14	47
1	k	216/263 (82%)	195 (90%)	20 (9%)	1 (0%)	24	59
1	o	216/263 (82%)	192 (89%)	22 (10%)	2 (1%)	14	47
1	s	217/263 (82%)	192 (88%)	23 (11%)	2 (1%)	14	47
1	w	219/263 (83%)	197 (90%)	22 (10%)	0	100	100
2	2	247/263 (94%)	228 (92%)	17 (7%)	2 (1%)	16	50
2	5	240/263 (91%)	220 (92%)	19 (8%)	1 (0%)	30	62
2	9	222/263 (84%)	198 (89%)	24 (11%)	0	100	100
2	AD	228/263 (87%)	209 (92%)	18 (8%)	1 (0%)	30	62
2	AH	227/263 (86%)	209 (92%)	16 (7%)	2 (1%)	14	47
2	AL	233/263 (89%)	210 (90%)	21 (9%)	2 (1%)	14	47
2	AP	222/263 (84%)	202 (91%)	16 (7%)	4 (2%)	6	34
2	B	249/263 (95%)	230 (92%)	19 (8%)	0	100	100
2	F	247/263 (94%)	223 (90%)	24 (10%)	0	100	100
2	J	247/263 (94%)	228 (92%)	19 (8%)	0	100	100
2	N	249/263 (95%)	225 (90%)	24 (10%)	0	100	100
2	R	247/263 (94%)	226 (92%)	19 (8%)	2 (1%)	16	50
2	V	248/263 (94%)	230 (93%)	18 (7%)	0	100	100
2	Z	247/263 (94%)	233 (94%)	14 (6%)	0	100	100
2	d	247/263 (94%)	231 (94%)	16 (6%)	0	100	100
2	h	248/263 (94%)	228 (92%)	19 (8%)	1 (0%)	30	62
2	l	227/263 (86%)	205 (90%)	16 (7%)	6 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	p	227/263 (86%)	205 (90%)	20 (9%)	2 (1%)	14	47
2	t	226/263 (86%)	208 (92%)	14 (6%)	4 (2%)	6	34
2	x	230/263 (88%)	211 (92%)	17 (7%)	2 (1%)	14	47
3	3	236/238 (99%)	220 (93%)	14 (6%)	2 (1%)	16	50
3	6	234/238 (98%)	216 (92%)	18 (8%)	0	100	100
3	AA	232/238 (98%)	209 (90%)	23 (10%)	0	100	100
3	AE	232/238 (98%)	210 (90%)	22 (10%)	0	100	100
3	AI	234/238 (98%)	212 (91%)	21 (9%)	1 (0%)	30	62
3	AM	232/238 (98%)	206 (89%)	26 (11%)	0	100	100
3	AQ	232/238 (98%)	206 (89%)	26 (11%)	0	100	100
3	C	236/238 (99%)	220 (93%)	16 (7%)	0	100	100
3	G	236/238 (99%)	218 (92%)	17 (7%)	1 (0%)	30	62
3	K	236/238 (99%)	222 (94%)	14 (6%)	0	100	100
3	O	236/238 (99%)	222 (94%)	14 (6%)	0	100	100
3	S	236/238 (99%)	219 (93%)	17 (7%)	0	100	100
3	W	236/238 (99%)	217 (92%)	19 (8%)	0	100	100
3	a	236/238 (99%)	219 (93%)	17 (7%)	0	100	100
3	e	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
3	i	236/238 (99%)	219 (93%)	17 (7%)	0	100	100
3	m	236/238 (99%)	215 (91%)	19 (8%)	2 (1%)	16	50
3	q	232/238 (98%)	212 (91%)	19 (8%)	1 (0%)	30	62
3	u	231/238 (97%)	207 (90%)	22 (10%)	2 (1%)	14	47
3	y	236/238 (99%)	213 (90%)	22 (9%)	1 (0%)	30	62
4	4	15/69 (22%)	15 (100%)	0	0	100	100
4	D	14/69 (20%)	14 (100%)	0	0	100	100
4	H	15/69 (22%)	15 (100%)	0	0	100	100
4	L	15/69 (22%)	14 (93%)	1 (7%)	0	100	100
4	P	14/69 (20%)	13 (93%)	1 (7%)	0	100	100
4	T	15/69 (22%)	15 (100%)	0	0	100	100
4	X	14/69 (20%)	12 (86%)	2 (14%)	0	100	100
4	b	13/69 (19%)	13 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	f	16/69 (23%)	14 (88%)	2 (12%)	0	100	100
4	j	15/69 (22%)	13 (87%)	2 (13%)	0	100	100
All	All	13969/15970 (88%)	12790 (92%)	1122 (8%)	57 (0%)	30	62

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	26	GLN
1	E	66	ASN
1	Q	69	GLU
2	l	16	ILE
2	l	21	SER

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	180/234 (77%)	180 (100%)	0	100	100
1	1	192/234 (82%)	192 (100%)	0	100	100
1	8	174/234 (74%)	174 (100%)	0	100	100
1	A	197/234 (84%)	197 (100%)	0	100	100
1	AC	180/234 (77%)	180 (100%)	0	100	100
1	AG	178/234 (76%)	177 (99%)	1 (1%)	78	84
1	AK	178/234 (76%)	178 (100%)	0	100	100
1	AO	177/234 (76%)	177 (100%)	0	100	100
1	E	194/234 (83%)	194 (100%)	0	100	100
1	I	194/234 (83%)	194 (100%)	0	100	100
1	M	194/234 (83%)	194 (100%)	0	100	100
1	Q	195/234 (83%)	195 (100%)	0	100	100
1	U	194/234 (83%)	194 (100%)	0	100	100
1	Y	195/234 (83%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	194/234 (83%)	193 (100%)	1 (0%)	81	85
1	g	195/234 (83%)	195 (100%)	0	100	100
1	k	183/234 (78%)	183 (100%)	0	100	100
1	o	184/234 (79%)	183 (100%)	1 (0%)	81	85
1	s	183/234 (78%)	183 (100%)	0	100	100
1	w	180/234 (77%)	180 (100%)	0	100	100
2	2	209/226 (92%)	209 (100%)	0	100	100
2	5	191/226 (84%)	191 (100%)	0	100	100
2	9	184/226 (81%)	184 (100%)	0	100	100
2	AD	184/226 (81%)	184 (100%)	0	100	100
2	AH	182/226 (80%)	182 (100%)	0	100	100
2	AL	191/226 (84%)	191 (100%)	0	100	100
2	AP	173/226 (76%)	173 (100%)	0	100	100
2	B	213/226 (94%)	213 (100%)	0	100	100
2	F	208/226 (92%)	208 (100%)	0	100	100
2	J	209/226 (92%)	208 (100%)	1 (0%)	81	85
2	N	212/226 (94%)	212 (100%)	0	100	100
2	R	209/226 (92%)	209 (100%)	0	100	100
2	V	210/226 (93%)	210 (100%)	0	100	100
2	Z	211/226 (93%)	211 (100%)	0	100	100
2	d	210/226 (93%)	210 (100%)	0	100	100
2	h	211/226 (93%)	211 (100%)	0	100	100
2	l	186/226 (82%)	186 (100%)	0	100	100
2	p	192/226 (85%)	192 (100%)	0	100	100
2	t	190/226 (84%)	190 (100%)	0	100	100
2	x	190/226 (84%)	189 (100%)	1 (0%)	81	85
3	3	205/208 (99%)	205 (100%)	0	100	100
3	6	187/208 (90%)	187 (100%)	0	100	100
3	AA	188/208 (90%)	188 (100%)	0	100	100
3	AE	189/208 (91%)	189 (100%)	0	100	100
3	AI	192/208 (92%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AM	189/208 (91%)	189 (100%)	0	100	100
3	AQ	182/208 (88%)	182 (100%)	0	100	100
3	C	205/208 (99%)	205 (100%)	0	100	100
3	G	203/208 (98%)	203 (100%)	0	100	100
3	K	201/208 (97%)	201 (100%)	0	100	100
3	O	205/208 (99%)	205 (100%)	0	100	100
3	S	203/208 (98%)	203 (100%)	0	100	100
3	W	201/208 (97%)	201 (100%)	0	100	100
3	a	205/208 (99%)	205 (100%)	0	100	100
3	e	204/208 (98%)	204 (100%)	0	100	100
3	i	204/208 (98%)	204 (100%)	0	100	100
3	m	189/208 (91%)	189 (100%)	0	100	100
3	q	189/208 (91%)	189 (100%)	0	100	100
3	u	191/208 (92%)	191 (100%)	0	100	100
3	y	193/208 (93%)	193 (100%)	0	100	100
4	4	13/57 (23%)	13 (100%)	0	100	100
4	D	13/57 (23%)	13 (100%)	0	100	100
4	H	14/57 (25%)	14 (100%)	0	100	100
4	L	13/57 (23%)	13 (100%)	0	100	100
4	P	13/57 (23%)	13 (100%)	0	100	100
4	T	14/57 (25%)	14 (100%)	0	100	100
4	X	13/57 (23%)	13 (100%)	0	100	100
4	b	12/57 (21%)	12 (100%)	0	100	100
4	f	15/57 (26%)	15 (100%)	0	100	100
4	j	14/57 (25%)	14 (100%)	0	100	100
All	All	11765/13930 (84%)	11760 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	258	ARG
1	c	116	SER
1	o	61	TYR

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Mol	Chain	Res	Type
2	x	163	THR
1	AG	172	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
2	d	219	ASN
1	AO	183	GLN
3	q	61	ASN
1	AO	122	GLN
2	AH	198	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	MYR	A	301	-	15,15,15	0.77	1 (6%)	15,15,15	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MYR	M	301	-	15,15,15	0.76	1 (6%)	15,15,15	0.62	0
5	MYR	Q	301	-	15,15,15	0.78	1 (6%)	15,15,15	0.62	0
5	MYR	U	301	-	15,15,15	0.72	0	15,15,15	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MYR	A	301	-	-	8/13/13/13	-
5	MYR	M	301	-	-	6/13/13/13	-
5	MYR	Q	301	-	-	5/13/13/13	-
5	MYR	U	301	-	-	2/13/13/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	301	MYR	C2-C1	2.23	1.55	1.50
5	M	301	MYR	C2-C1	2.08	1.55	1.50
5	A	301	MYR	C2-C1	2.07	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	301	MYR	C6-C7-C8-C9
5	M	301	MYR	C3-C4-C5-C6
5	U	301	MYR	C11-C10-C9-C8
5	A	301	MYR	C4-C5-C6-C7
5	M	301	MYR	C9-C10-C11-C12

There are no ring outliers.

3 monomers are involved in 8 short contacts:

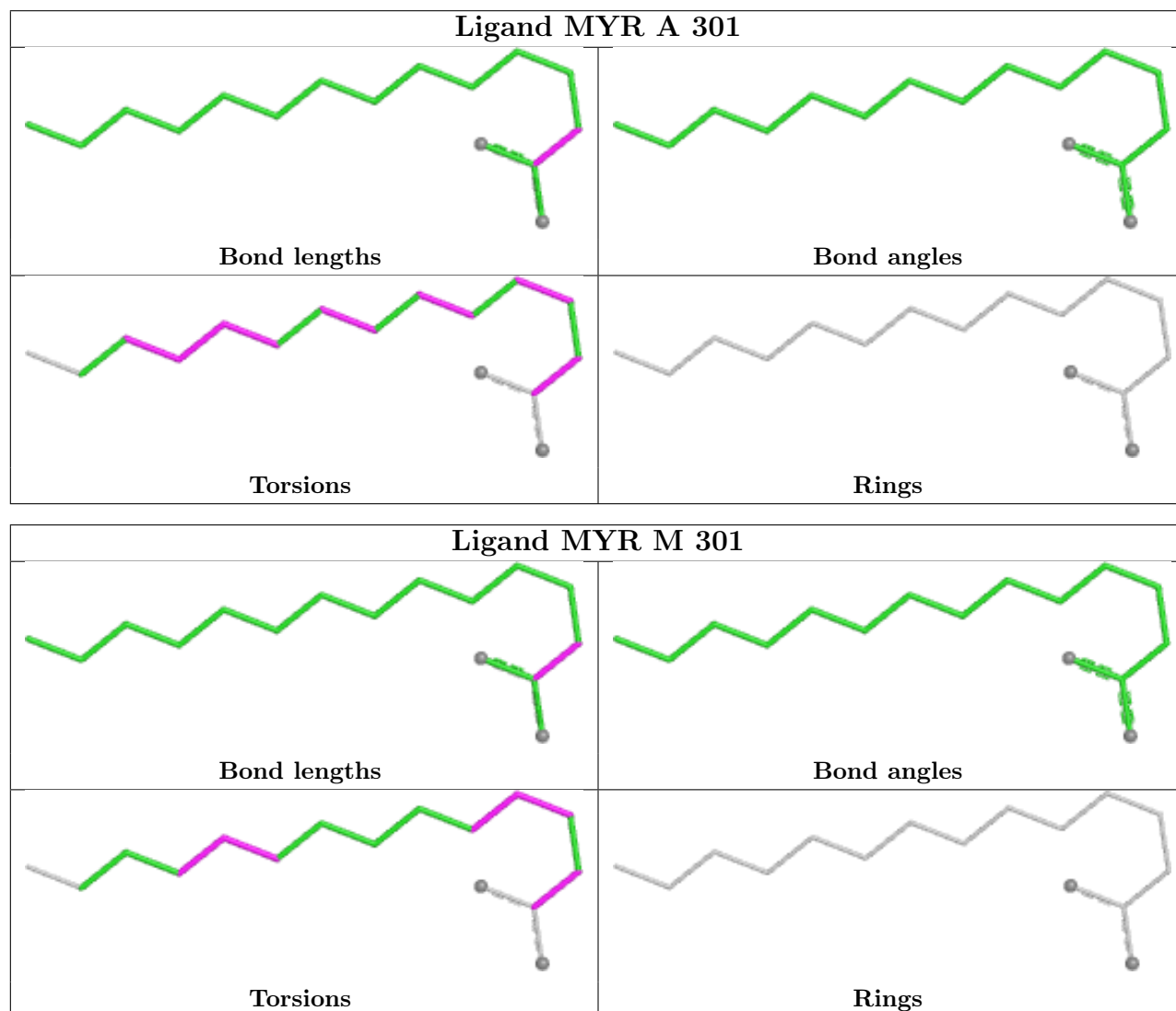
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	301	MYR	2	0
5	Q	301	MYR	2	0

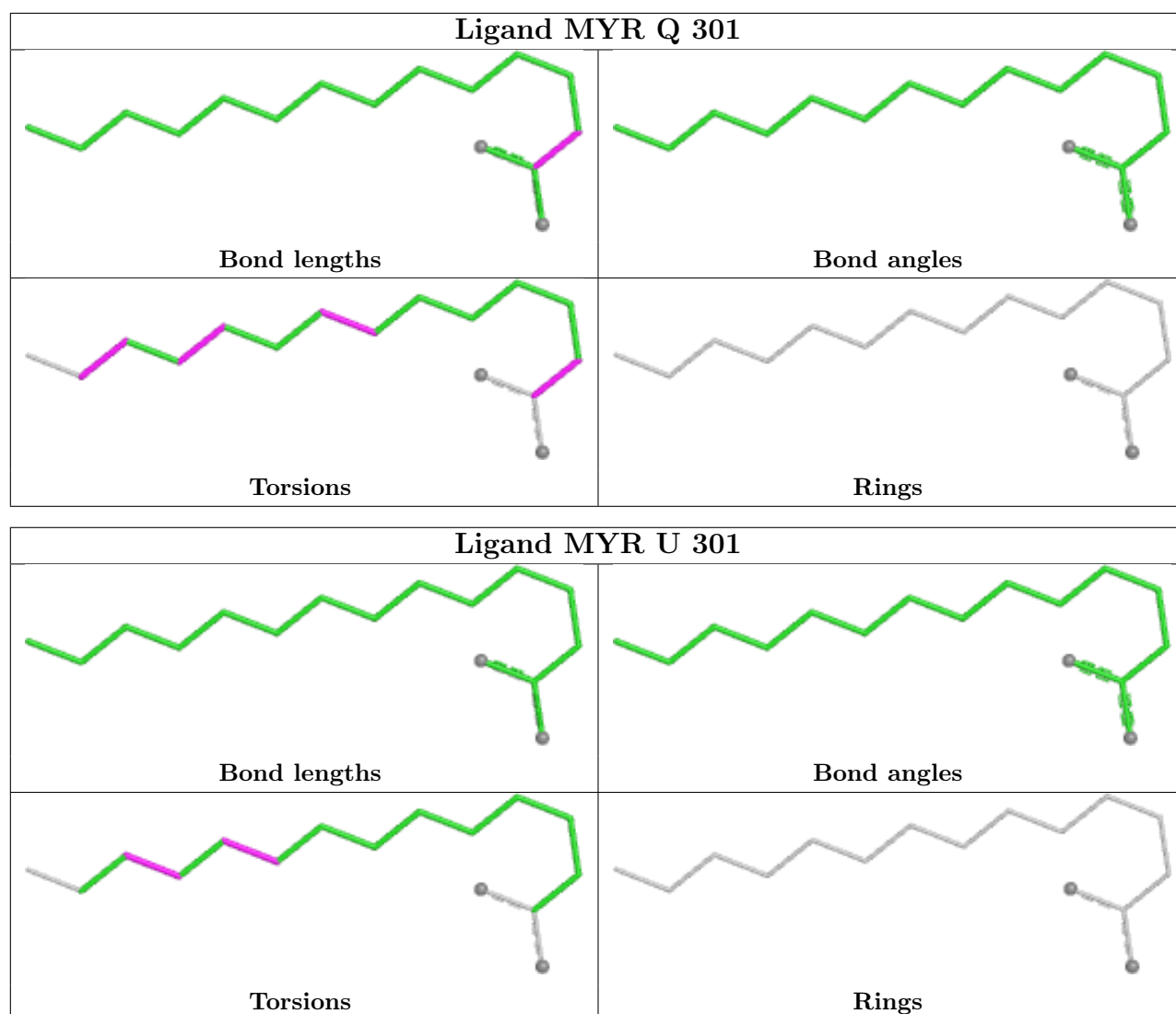
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	301	MYR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	217/263 (82%)	1.03	30 (13%) 6 5	97, 110, 132, 147	0
1	1	223/263 (84%)	0.55	11 (4%) 35 22	85, 96, 113, 143	0
1	8	218/263 (82%)	1.02	25 (11%) 9 7	103, 121, 147, 175	0
1	A	228/263 (86%)	0.49	9 (3%) 43 27	80, 94, 122, 183	0
1	AC	219/263 (83%)	0.99	27 (12%) 8 6	104, 122, 146, 162	0
1	AG	219/263 (83%)	1.08	30 (13%) 6 5	102, 119, 151, 174	0
1	AK	219/263 (83%)	0.93	32 (14%) 6 4	107, 121, 141, 164	0
1	AO	219/263 (83%)	1.06	31 (14%) 6 5	106, 122, 143, 165	0
1	E	222/263 (84%)	0.50	7 (3%) 50 31	84, 94, 112, 126	0
1	I	223/263 (84%)	0.45	7 (3%) 51 32	77, 93, 113, 135	0
1	M	222/263 (84%)	0.66	15 (6%) 23 15	78, 88, 111, 123	0
1	Q	222/263 (84%)	0.52	11 (4%) 34 22	74, 86, 107, 133	0
1	U	222/263 (84%)	0.49	5 (2%) 61 41	78, 88, 106, 126	0
1	Y	221/263 (84%)	0.41	7 (3%) 50 31	87, 95, 107, 133	0
1	c	222/263 (84%)	0.45	8 (3%) 46 28	82, 92, 116, 148	0
1	g	222/263 (84%)	0.51	7 (3%) 50 31	88, 96, 115, 135	0
1	k	218/263 (82%)	1.00	33 (15%) 5 4	92, 107, 130, 142	0
1	o	218/263 (82%)	0.86	21 (9%) 13 9	92, 109, 130, 143	0
1	s	219/263 (83%)	0.94	22 (10%) 12 8	93, 108, 134, 146	0
1	w	221/263 (84%)	1.02	37 (16%) 4 3	95, 110, 129, 144	0
2	2	249/263 (94%)	0.60	20 (8%) 18 12	75, 100, 127, 159	0
2	5	242/263 (92%)	0.97	35 (14%) 6 5	97, 115, 147, 185	0
2	9	226/263 (85%)	0.81	19 (8%) 17 11	89, 118, 142, 156	0
2	AD	232/263 (88%)	0.89	28 (12%) 8 6	99, 115, 151, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
2	AH	231/263 (87%)	0.91	32 (13%)	6	5	98, 114, 141, 160	0
2	AL	237/263 (90%)	0.98	34 (14%)	6	5	104, 124, 154, 203	0
2	AP	226/263 (85%)	1.00	33 (14%)	6	4	106, 120, 142, 205	0
2	B	251/263 (95%)	0.54	11 (4%)	39	24	81, 96, 124, 152	0
2	F	249/263 (94%)	0.64	22 (8%)	15	10	85, 95, 120, 150	0
2	J	249/263 (94%)	0.58	19 (7%)	20	13	85, 96, 118, 143	0
2	N	251/263 (95%)	0.57	14 (5%)	30	19	70, 92, 127, 206	0
2	R	249/263 (94%)	0.60	17 (6%)	23	15	77, 88, 107, 133	0
2	V	250/263 (95%)	0.71	22 (8%)	15	10	80, 93, 121, 143	0
2	Z	249/263 (94%)	0.55	15 (6%)	27	17	88, 102, 122, 149	0
2	d	249/263 (94%)	0.74	24 (9%)	13	9	83, 98, 127, 156	0
2	h	250/263 (95%)	0.69	22 (8%)	15	10	88, 101, 122, 153	0
2	l	231/263 (87%)	1.02	38 (16%)	4	3	95, 113, 140, 150	0
2	p	231/263 (87%)	0.83	30 (12%)	7	6	85, 106, 146, 172	0
2	t	230/263 (87%)	0.75	23 (10%)	12	8	92, 106, 134, 144	0
2	x	234/263 (88%)	0.80	18 (7%)	19	13	91, 112, 140, 192	0
3	3	238/238 (100%)	0.56	15 (6%)	26	17	87, 97, 109, 148	0
3	6	236/238 (99%)	1.01	41 (17%)	4	3	96, 115, 133, 157	0
3	AA	234/238 (98%)	1.06	36 (15%)	5	4	91, 122, 137, 152	0
3	AE	234/238 (98%)	1.01	38 (16%)	4	3	101, 121, 138, 171	0
3	AI	236/238 (99%)	0.88	28 (11%)	9	6	101, 119, 141, 173	0
3	AM	234/238 (98%)	1.08	41 (17%)	4	3	104, 119, 136, 151	0
3	AQ	234/238 (98%)	1.04	34 (14%)	6	5	102, 123, 142, 180	0
3	C	238/238 (100%)	0.62	17 (7%)	22	14	84, 96, 110, 153	0
3	G	238/238 (100%)	0.57	9 (3%)	44	27	86, 94, 108, 137	0
3	K	238/238 (100%)	0.60	13 (5%)	30	19	79, 94, 109, 170	0
3	O	238/238 (100%)	0.60	13 (5%)	30	19	82, 91, 103, 171	0
3	S	238/238 (100%)	0.60	13 (5%)	30	19	80, 88, 103, 184	0
3	W	238/238 (100%)	0.59	13 (5%)	30	19	75, 88, 102, 132	0
3	a	238/238 (100%)	0.64	9 (3%)	44	27	86, 95, 111, 143	0
3	e	238/238 (100%)	0.59	12 (5%)	34	22	80, 95, 111, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	i	238/238 (100%)	0.65	16 (6%) 24 15	90, 99, 116, 184	0
3	m	238/238 (100%)	1.11	41 (17%) 4 3	95, 112, 131, 145	0
3	q	234/238 (98%)	0.95	28 (11%) 9 6	93, 108, 128, 148	0
3	u	233/238 (97%)	0.93	27 (11%) 9 7	93, 108, 133, 145	0
3	y	238/238 (100%)	0.89	31 (13%) 7 6	90, 110, 130, 149	0
4	4	17/69 (24%)	0.46	1 (5%) 28 18	99, 105, 125, 127	0
4	D	16/69 (23%)	0.04	0 100 100	97, 103, 121, 130	0
4	H	17/69 (24%)	0.20	1 (5%) 28 18	92, 103, 135, 142	0
4	L	17/69 (24%)	0.74	1 (5%) 28 18	99, 107, 133, 135	0
4	P	16/69 (23%)	0.20	0 100 100	88, 98, 121, 133	0
4	T	17/69 (24%)	0.51	0 100 100	89, 97, 123, 132	0
4	X	16/69 (23%)	0.22	0 100 100	89, 97, 109, 118	0
4	b	15/69 (21%)	0.39	1 (6%) 24 15	98, 109, 127, 130	0
4	f	18/69 (26%)	0.45	1 (5%) 30 19	95, 108, 150, 172	0
4	j	17/69 (24%)	0.33	1 (5%) 28 18	100, 109, 136, 138	0
All	All	14127/15970 (88%)	0.76	1332 (9%) 14 9	70, 104, 135, 206	0

The worst 5 of 1332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AL	46	GLU	11.2
3	AA	78	ASN	8.4
3	u	185	THR	7.7
2	l	60	THR	7.0
3	G	1	GLY	6.9

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

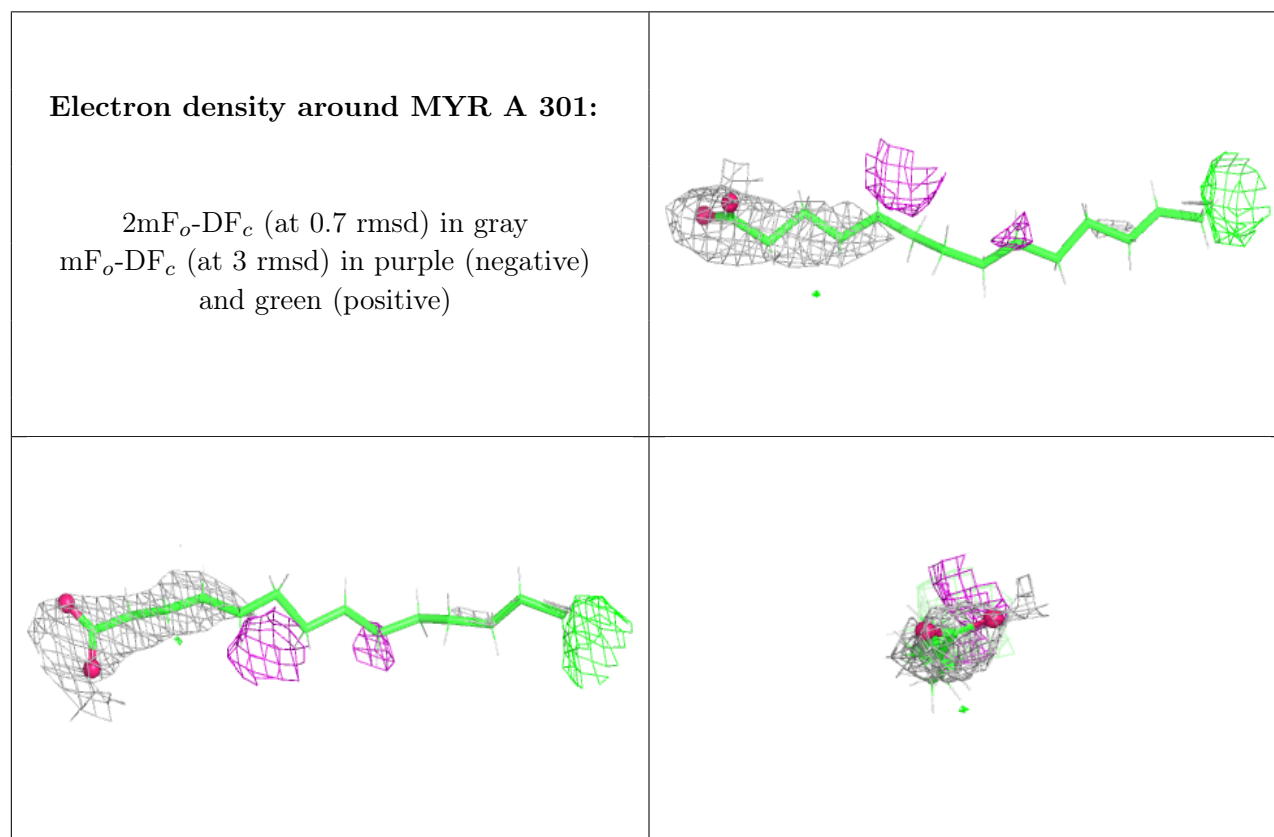
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MYR	A	301	16/16	0.86	0.25	62,76,80,80	0
5	MYR	M	301	16/16	0.88	0.26	59,72,76,76	0
5	MYR	Q	301	16/16	0.89	0.25	58,71,75,77	0
5	MYR	U	301	16/16	0.90	0.23	59,72,76,76	0

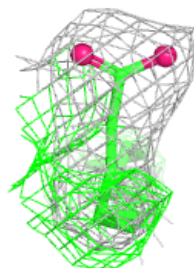
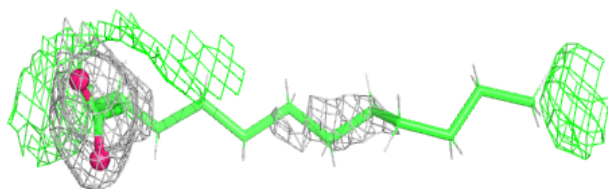
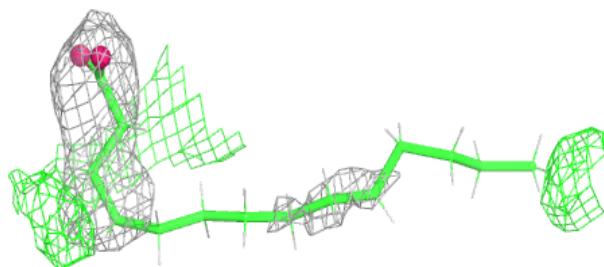
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



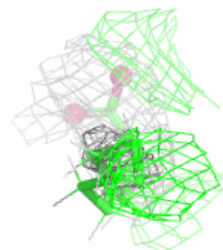
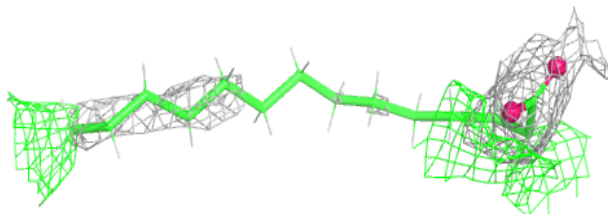
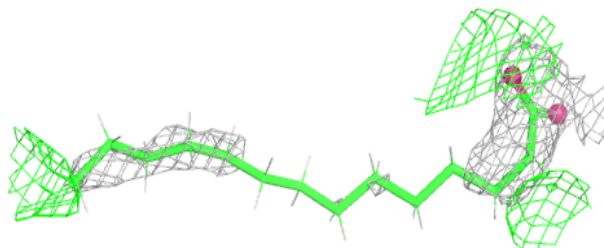


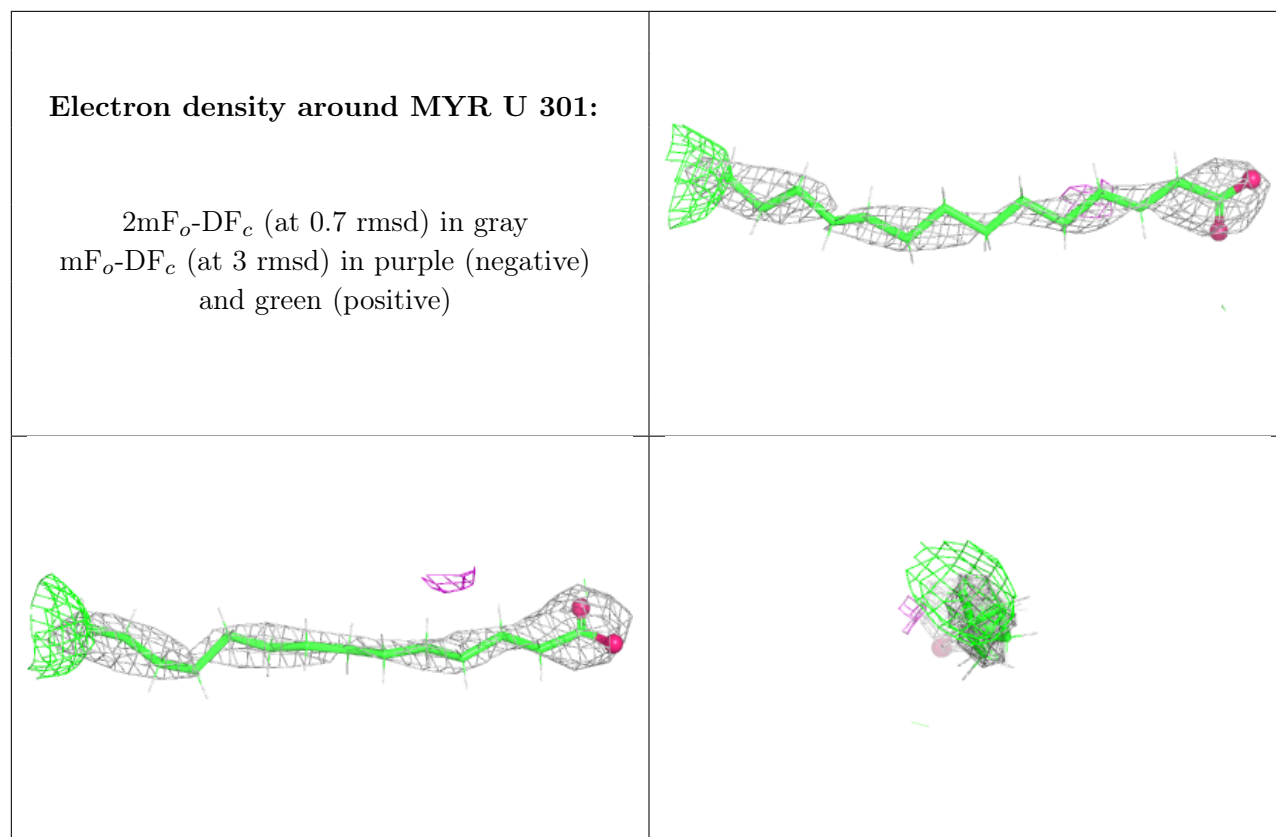
**Electron density around MYR M 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MYR Q 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.