



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 04:19 am BST

PDB ID : 3PHF  
Title : Crystal Structure of the Epstein-Barr virus gH and gL complex  
Authors : Matsuura, H.; Kirschner, A.N.; Jardetzky, T.S.  
Deposited on : 2010-11-04  
Resolution : 3.58 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

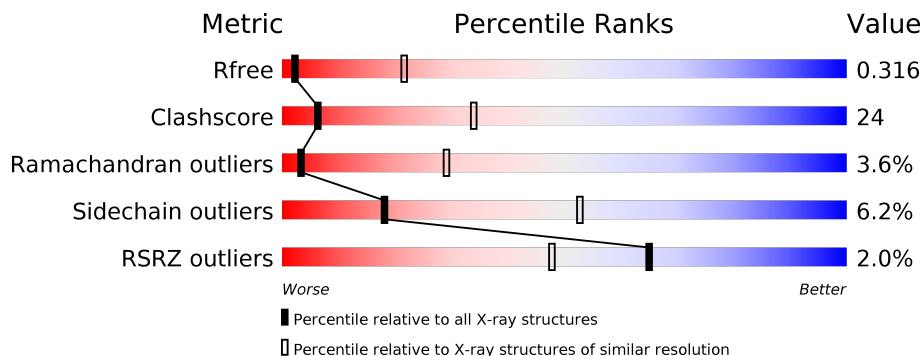
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.58 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.




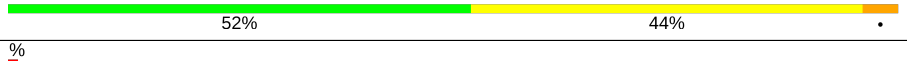

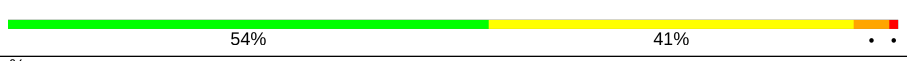



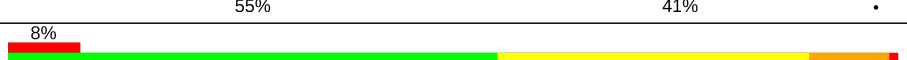

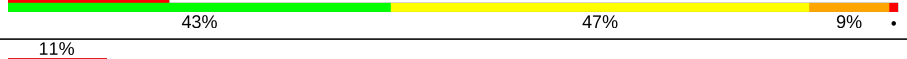


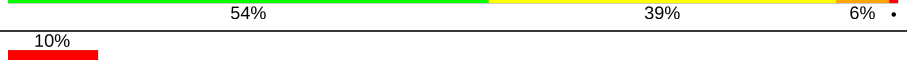
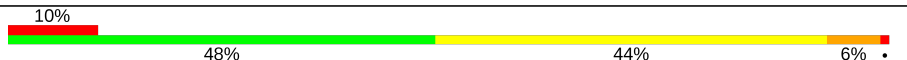



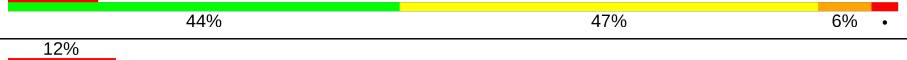



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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 on 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	1	653	
1	3	653	
1	5	653	
1	A	653	
1	C	653	
1	E	653	


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Mol	Chain	Length	Quality of chain
1	G	653	 % 54% 43%
1	I	653	 % 52% 44%
1	K	653	 % 55% 42%
1	M	653	 % 53% 43%
1	O	653	 % 54% 41%
1	Q	653	 % 53% 43%
1	S	653	 % 54% 41% 5%
1	U	653	 % 53% 43%
1	W	653	 % 55% 40% 5%
1	Y	653	 % 55% 41%
2	2	108	 8% 55% 35% 9%
2	4	108	 17% 50% 43% 6%
2	6	108	 18% 43% 47% 9%
2	B	108	 11% 51% 43% 6%
2	D	108	 4% 50% 41% 6%
2	F	108	 9% 48% 42% 8%
2	H	108	 9% 54% 39% 6%
2	J	108	 10% 50% 41% 7%
2	L	108	 10% 48% 44% 6%
2	N	108	 4% 48% 44% 6%
2	P	108	 7% 51% 37% 11%
2	R	108	12% 52% 41% 6%
2	T	108	4% 45% 44% 10%
2	V	108	10% 44% 47% 6%
2	X	108	12% 53% 38% 8%

Continued on next page...

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Mol	Chain	Length	Quality of chain
2	Z	108	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '14%', a green segment in the middle labeled '48%', and a yellow segment on the right labeled '46%'. At the far right end of the bar, there are two small black dots.</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 94656 atoms, of which 0 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	653	5078	3253	840	954	31	0	0	0
1	C	653	5078	3253	840	954	31	0	0	0
1	E	653	5078	3253	840	954	31	0	0	0
1	G	653	5078	3253	840	954	31	0	0	0
1	I	653	5078	3253	840	954	31	0	0	0
1	K	653	5078	3253	840	954	31	0	0	0
1	M	653	5078	3253	840	954	31	0	0	0
1	O	653	5078	3253	840	954	31	0	0	0
1	Q	653	5078	3253	840	954	31	0	0	0
1	S	653	5078	3253	840	954	31	0	0	0
1	U	653	5078	3253	840	954	31	0	0	0
1	W	653	5078	3253	840	954	31	0	0	0
1	Y	653	5078	3253	840	954	31	0	0	0
1	1	653	5078	3253	840	954	31	0	0	0
1	3	653	5078	3253	840	954	31	0	0	0
1	5	653	5078	3253	840	954	31	0	0	0

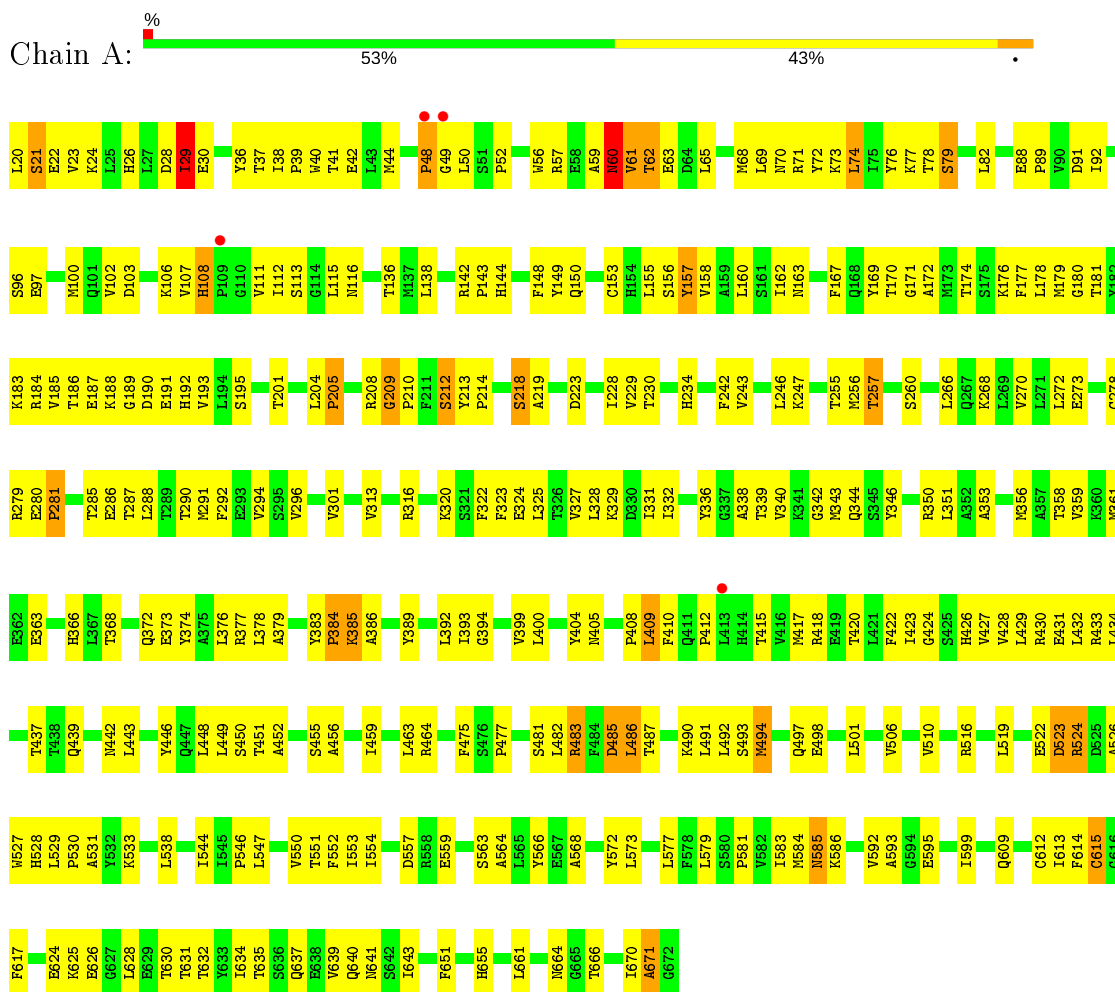
- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	D	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	F	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	H	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	J	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	L	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	N	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	P	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	R	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	T	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	V	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	X	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	Z	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	2	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	4	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			
2	6	108	Total	C	N	O	S	0	0	0
			838	529	145	160	4			

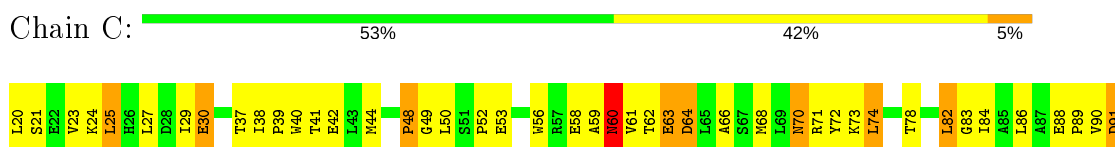
### 3 Residue-property plots

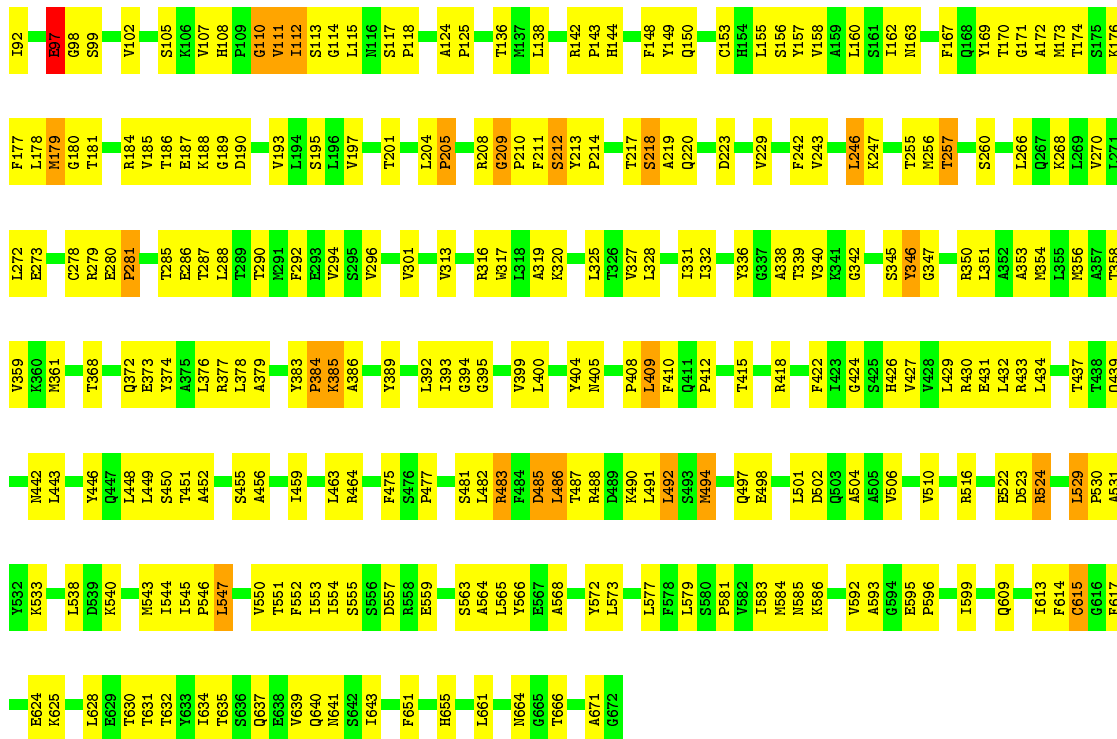
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Envelope glycoprotein H

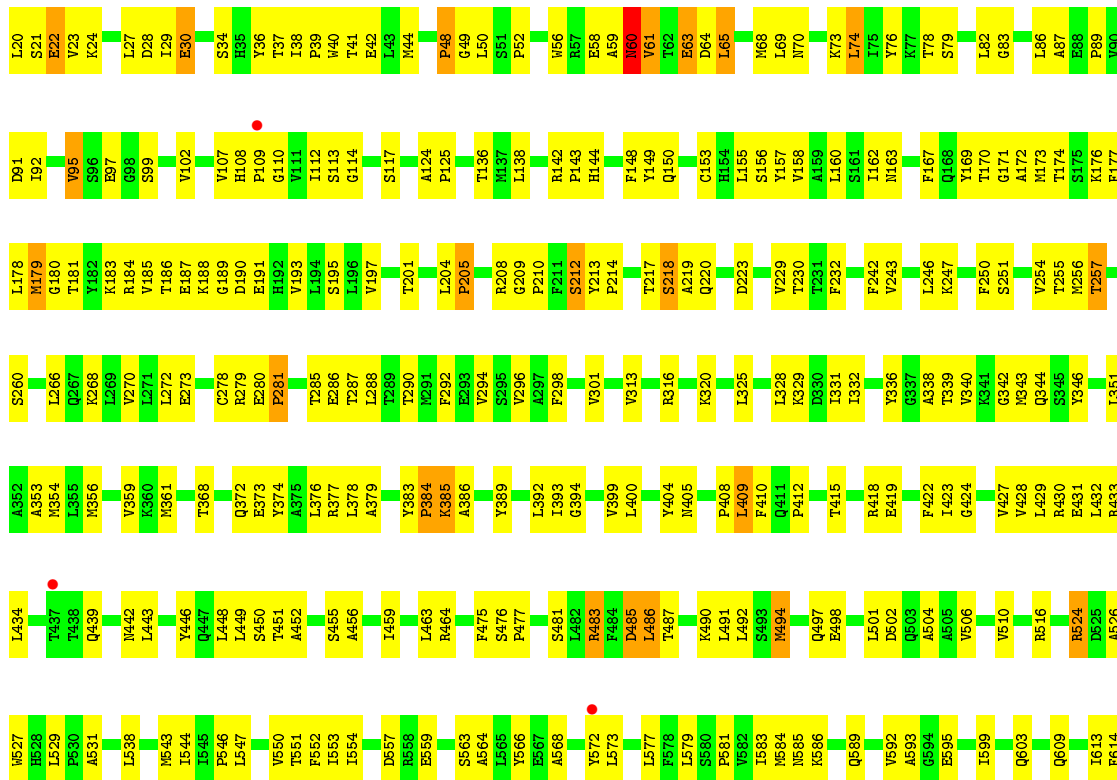


- Molecule 1: Envelope glycoprotein H





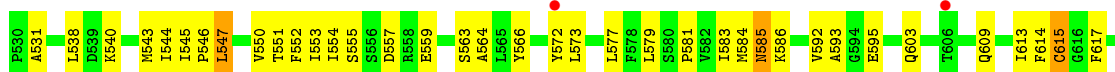
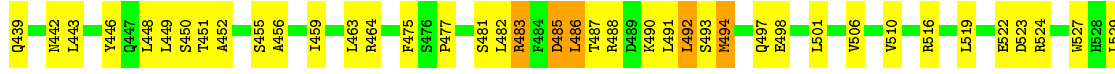
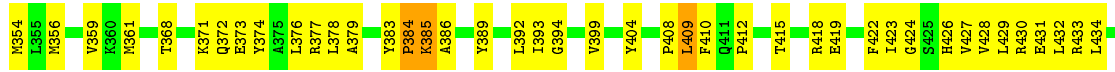
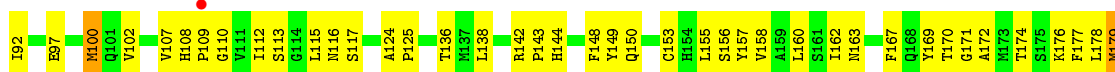
● Molecule 1: Envelope glycoprotein H



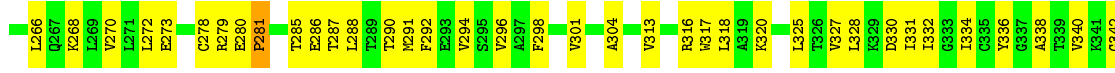


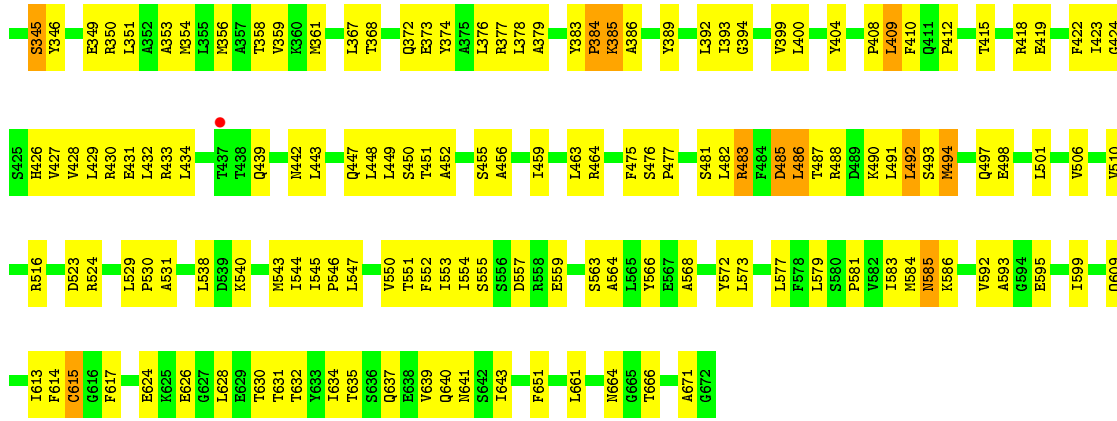


● Molecule 1: Envelope glycoprotein H

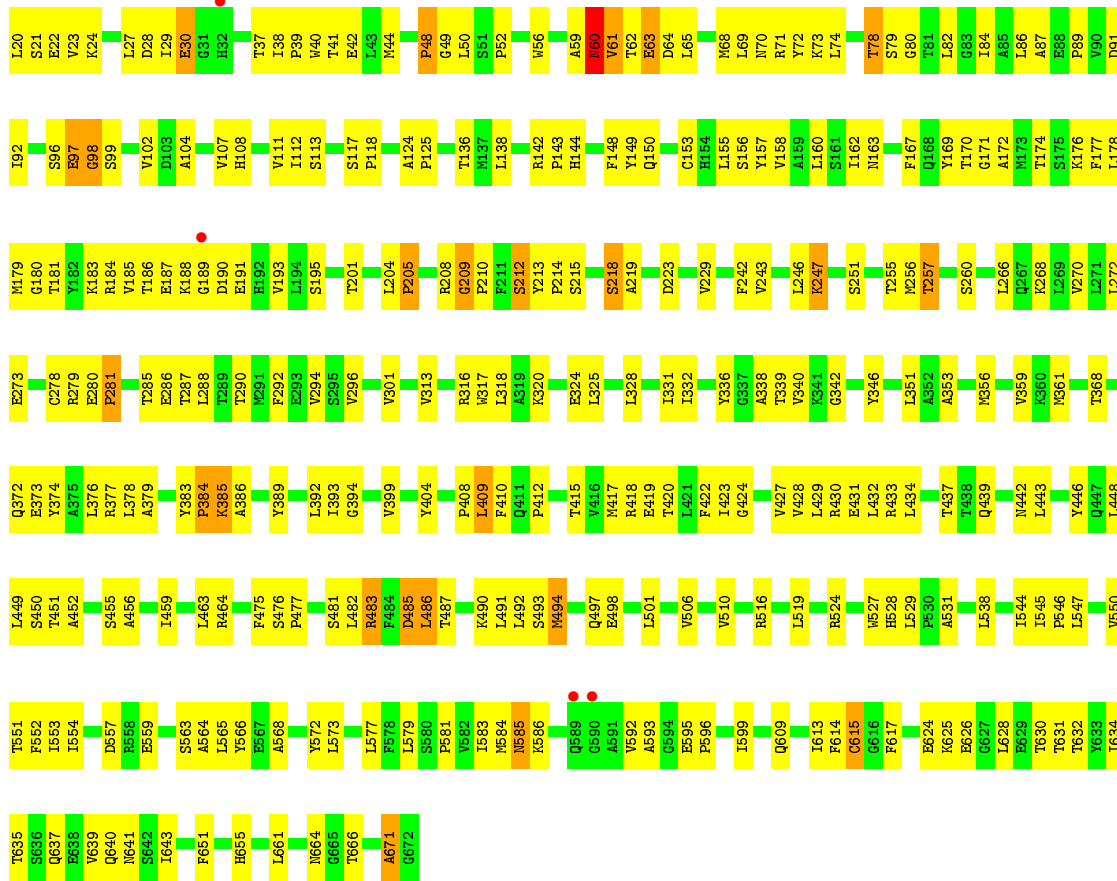


● Molecule 1: Envelope glycoprotein H



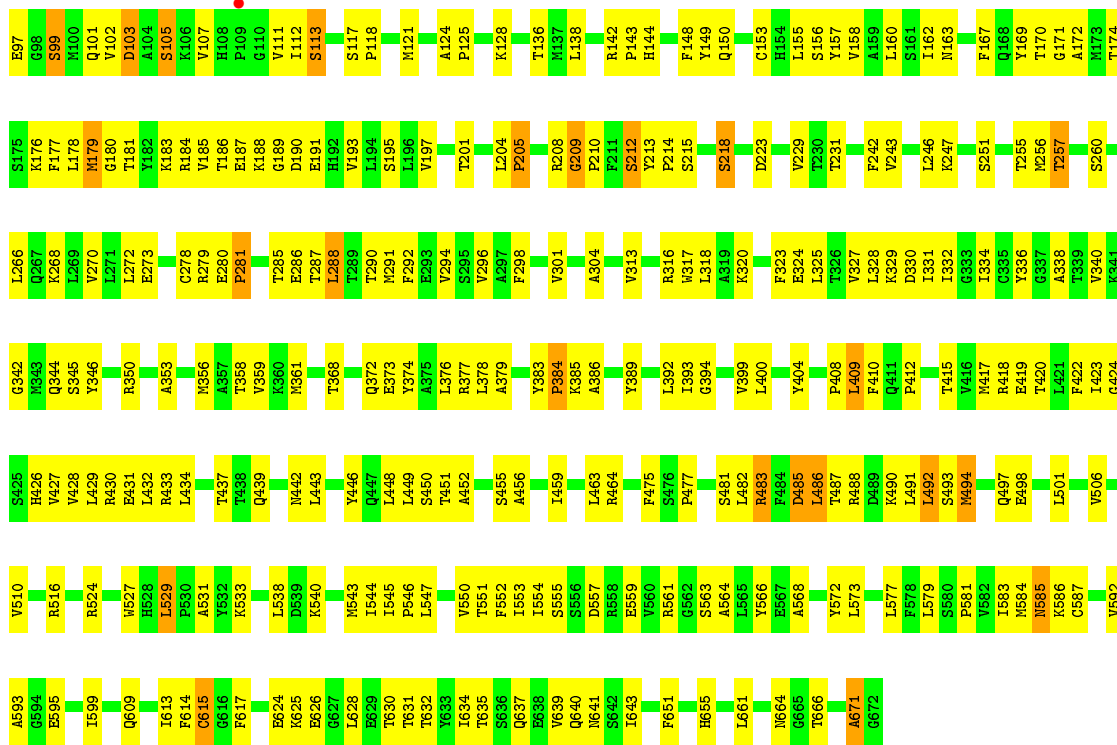


• Molecule 1: Envelope glycoprotein H

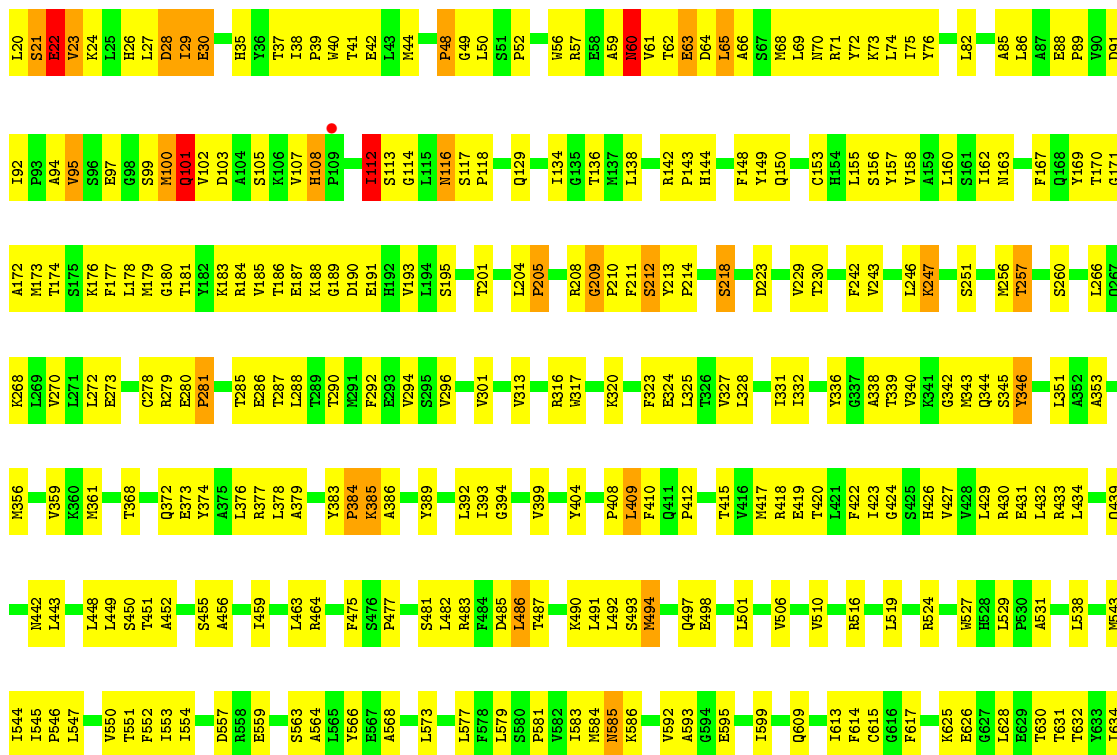


• Molecule 1: Envelope glycoprotein H



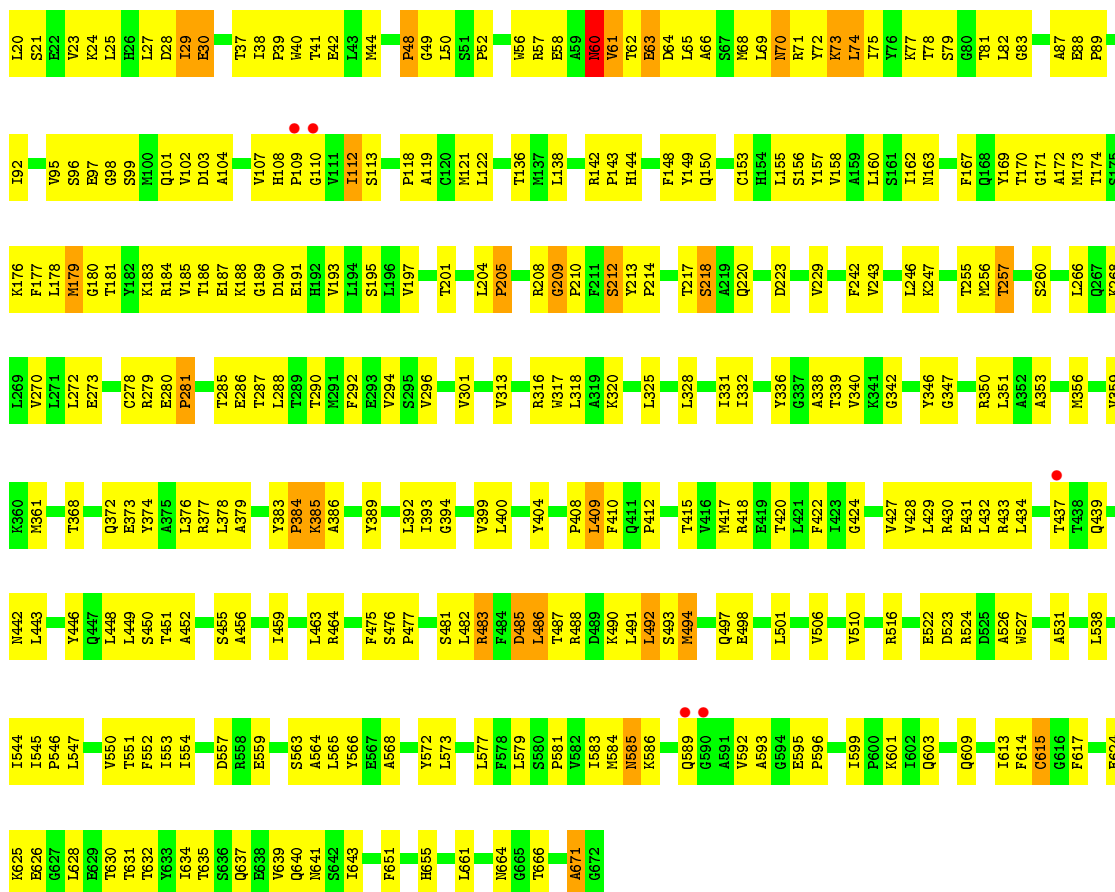


• Molecule 1: Envelope glycoprotein H

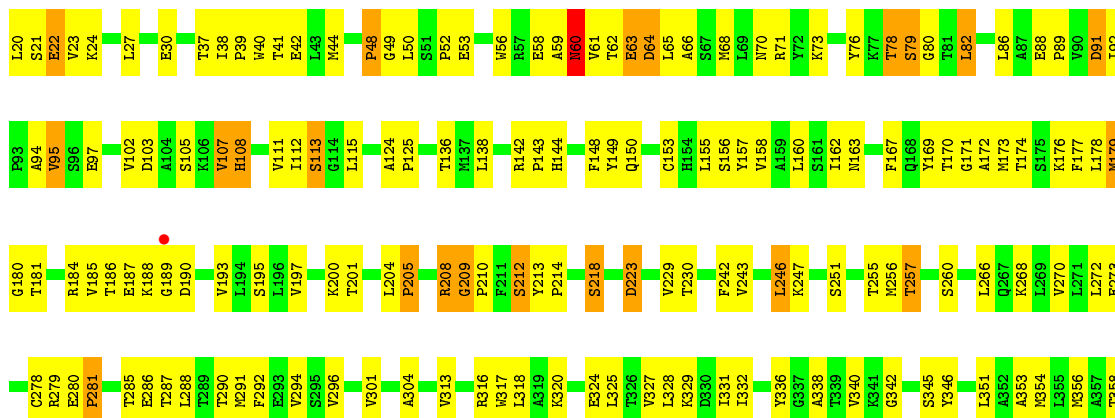


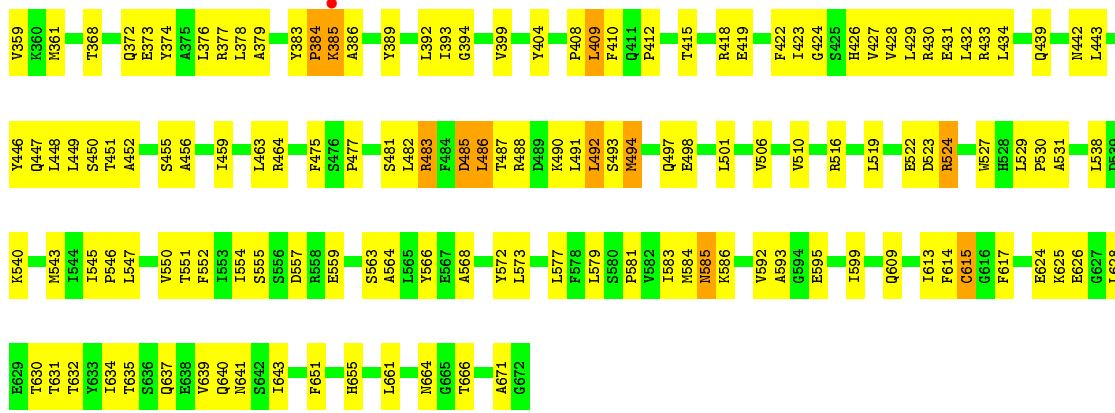


● Molecule 1: Envelope glycoprotein H

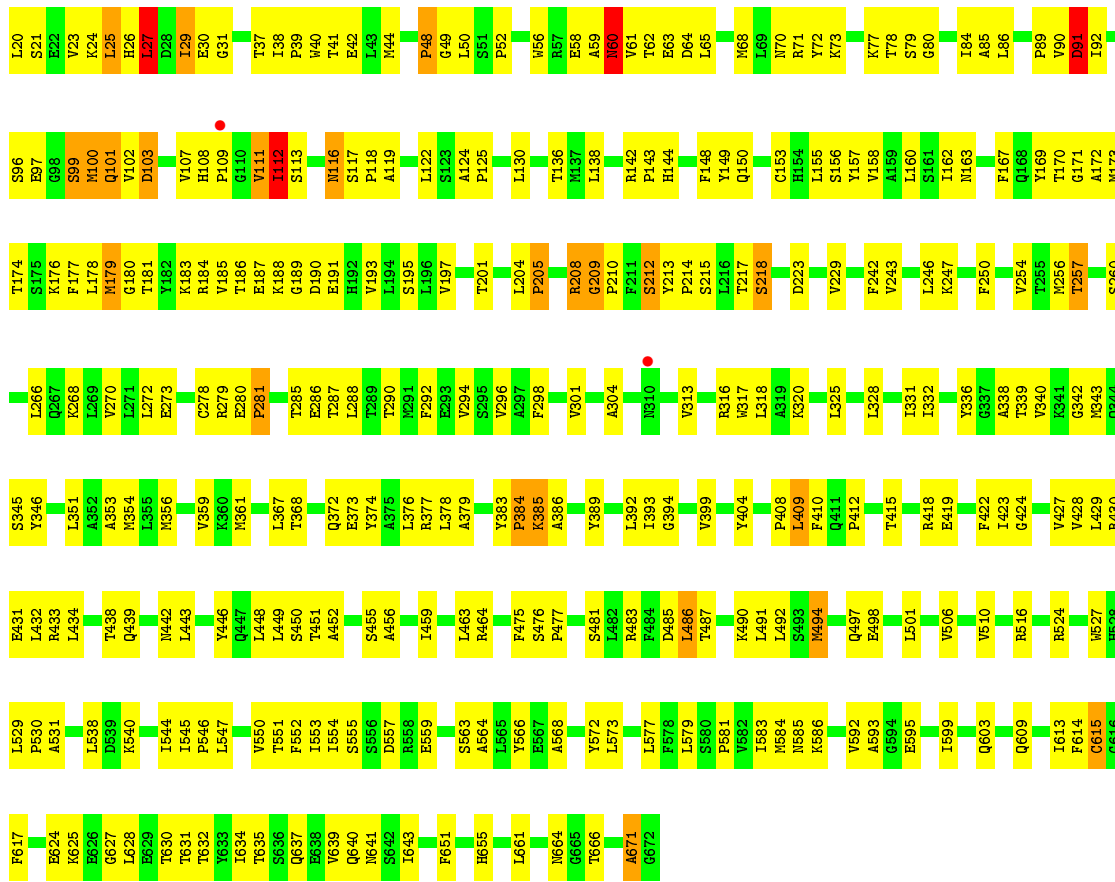


● Molecule 1: Envelope glycoprotein H

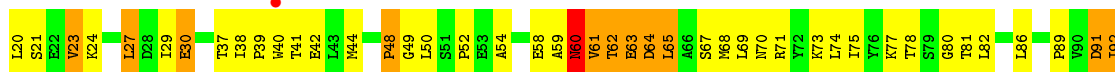


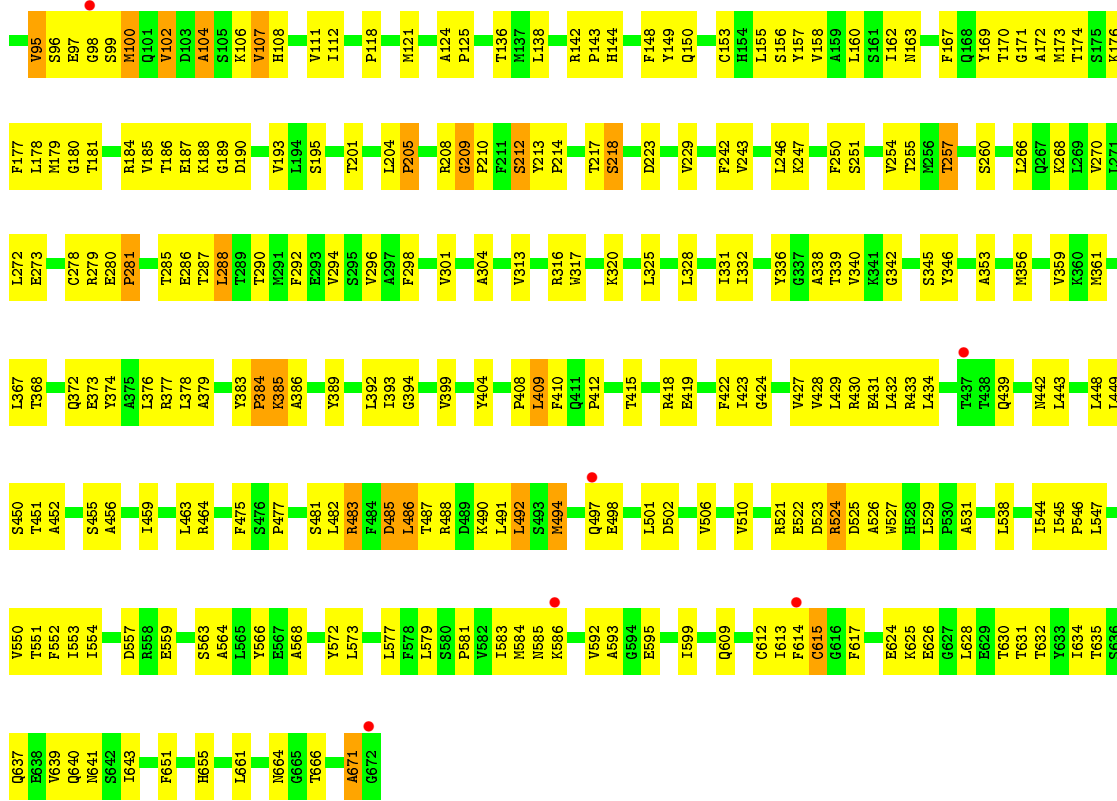


● Molecule 1: Envelope glycoprotein H

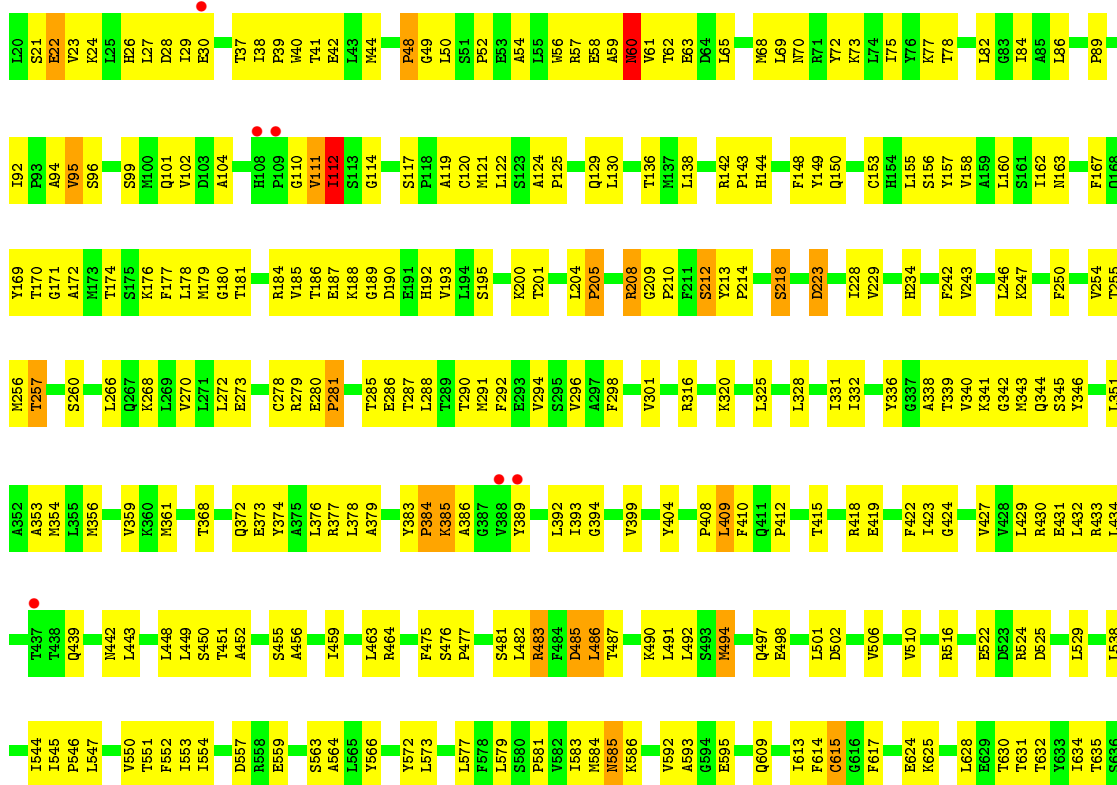


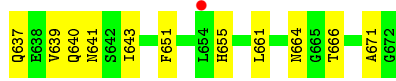
● Molecule 1: Envelope glycoprotein H



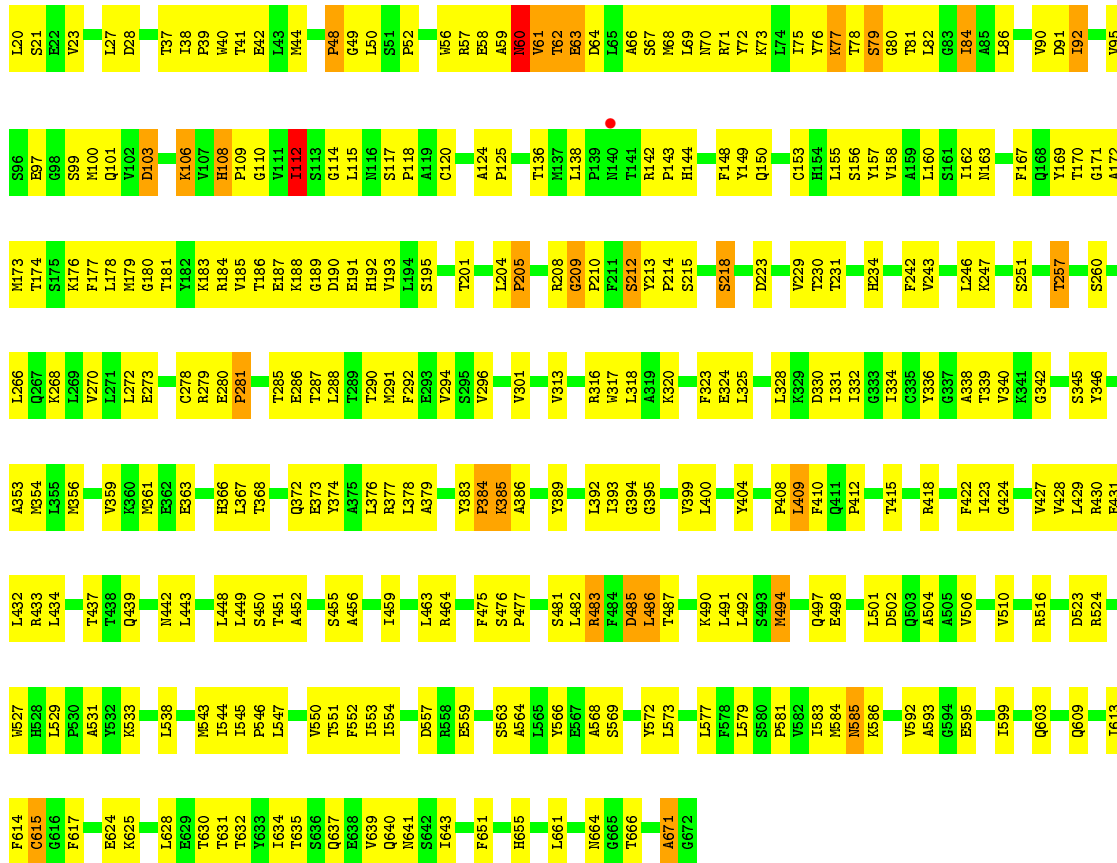


● Molecule 1: Envelope glycoprotein H

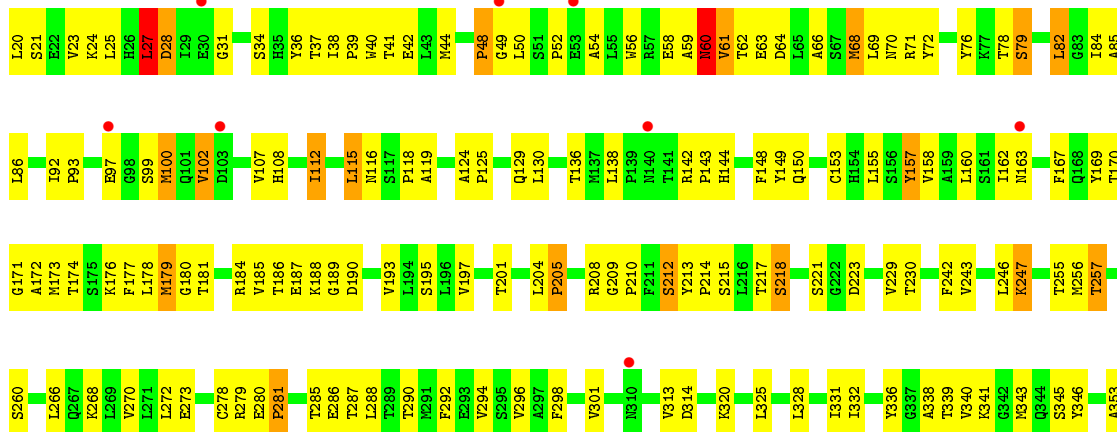


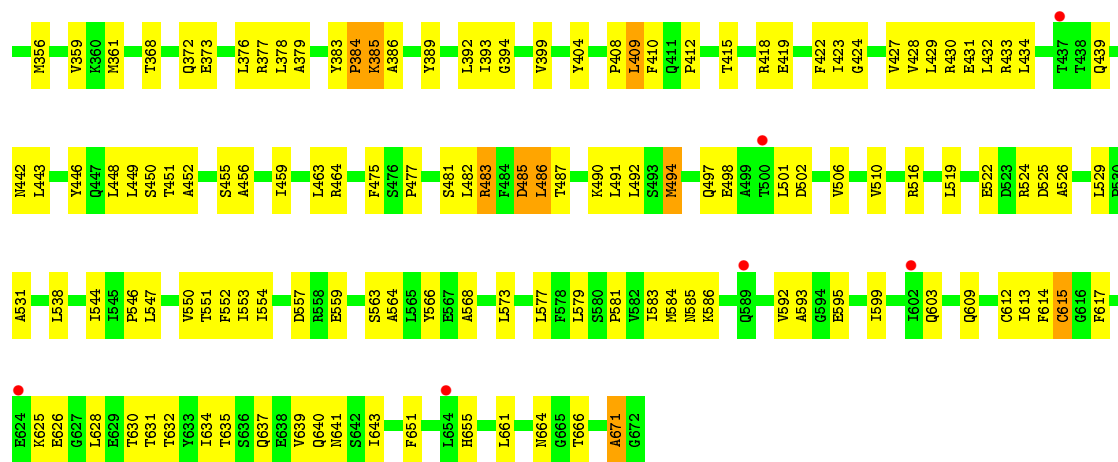


• Molecule 1: Envelope glycoprotein H

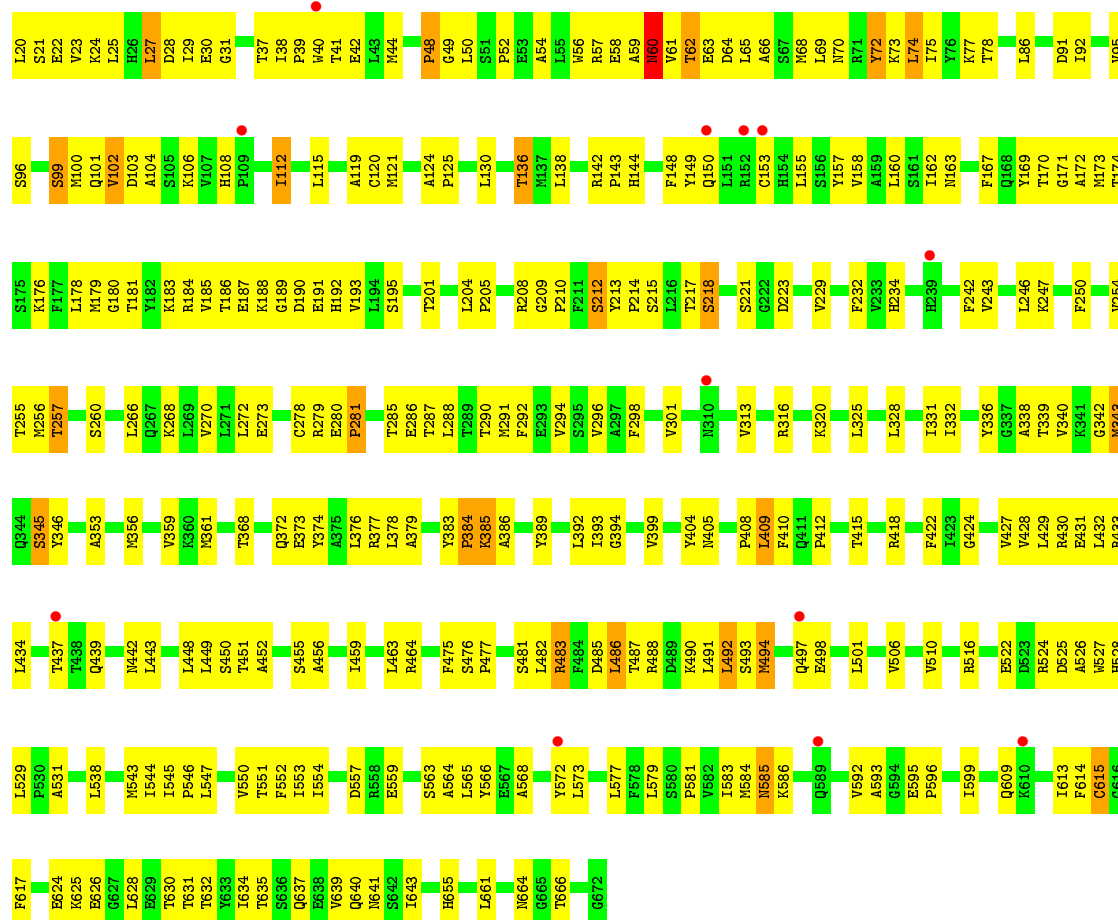


• Molecule 1: Envelope glycoprotein H





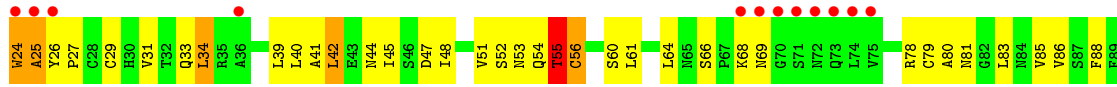
• Molecule 1: Envelope glycoprotein H



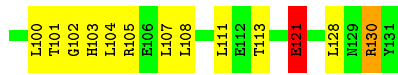
• Molecule 2: Envelope glycoprotein L



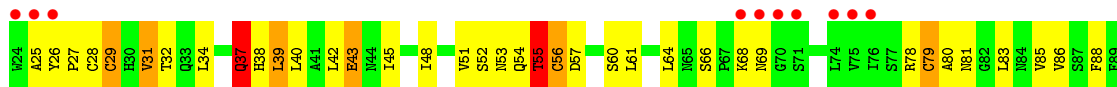




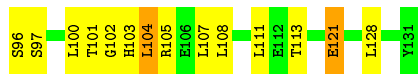
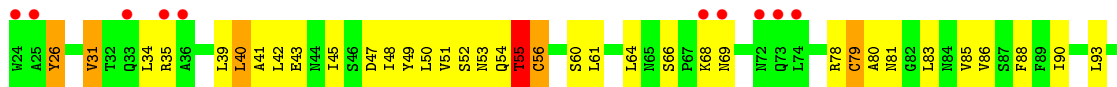
• Molecule 2: Envelope glycoprotein L



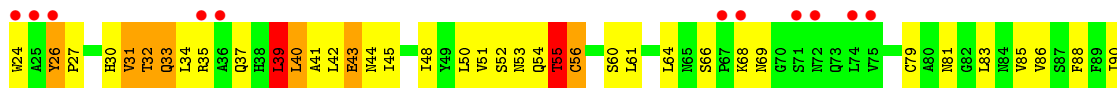
• Molecule 2: Envelope glycoprotein L



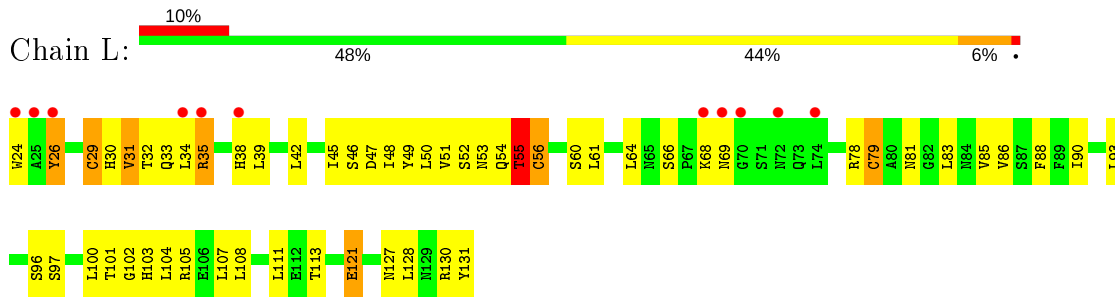
• Molecule 2: Envelope glycoprotein L



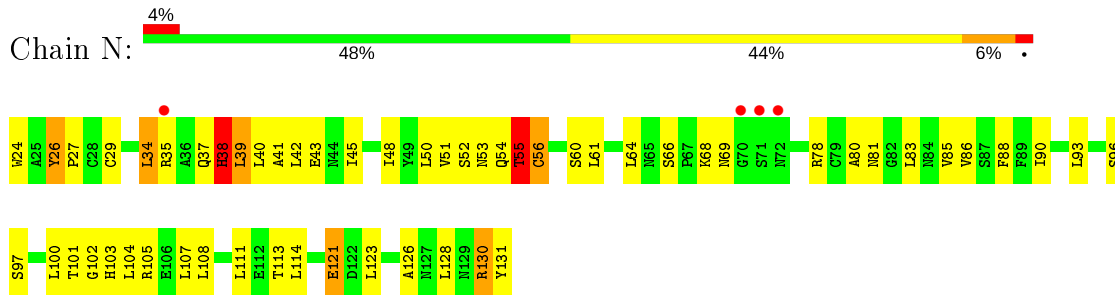
• Molecule 2: Envelope glycoprotein L



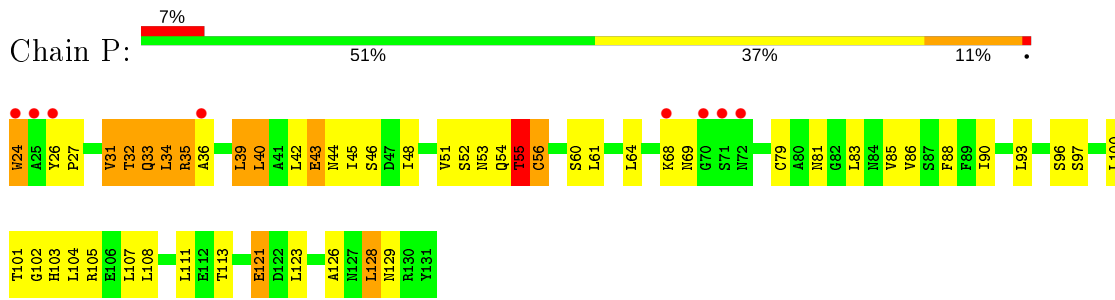
• Molecule 2: Envelope glycoprotein L



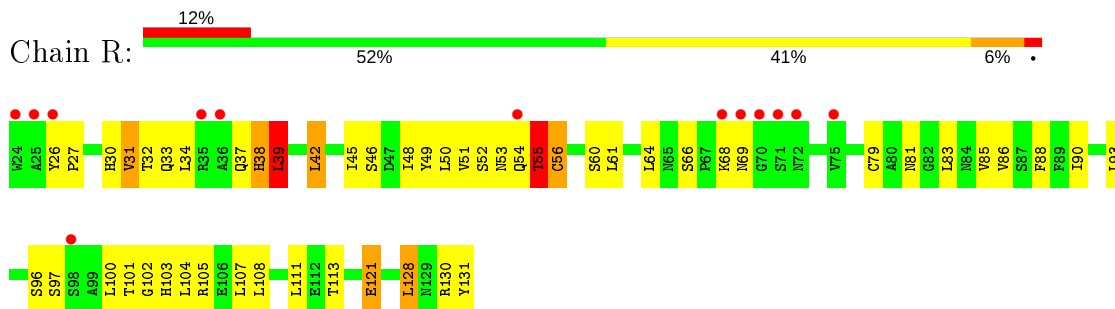
• Molecule 2: Envelope glycoprotein L



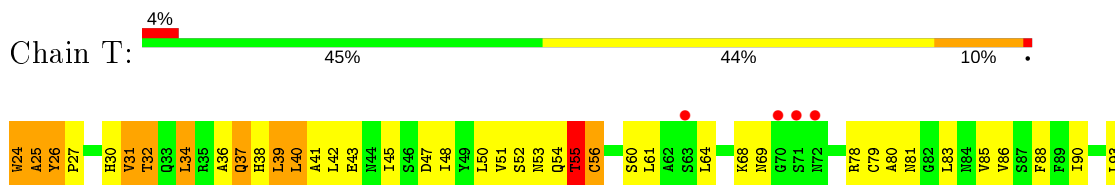
• Molecule 2: Envelope glycoprotein L



• Molecule 2: Envelope glycoprotein L



• Molecule 2: Envelope glycoprotein L

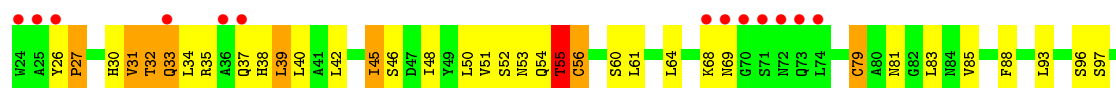




- Molecule 2: Envelope glycoprotein L



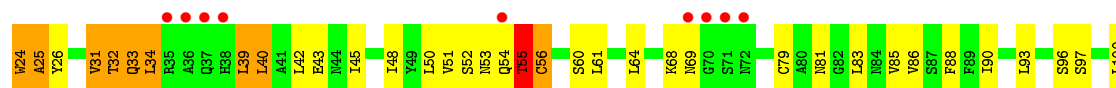
- Molecule 2: Envelope glycoprotein L



- Molecule 2: Envelope glycoprotein L

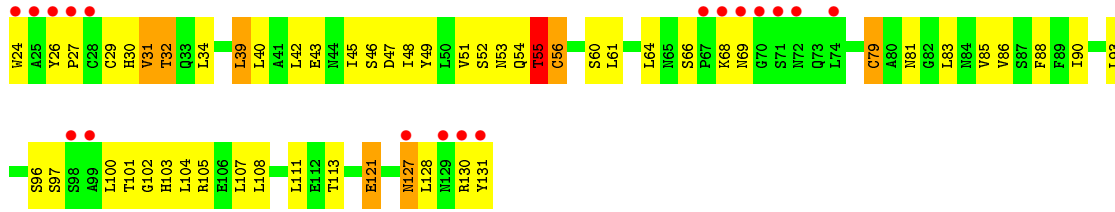


- Molecule 2: Envelope glycoprotein L

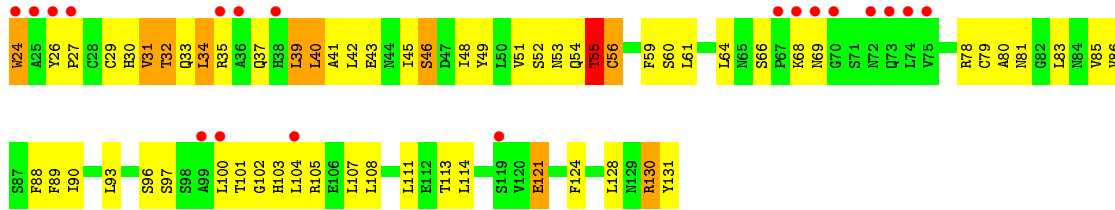


- Molecule 2: Envelope glycoprotein L





● Molecule 2: Envelope glycoprotein L



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.51Å 244.91Å 287.95Å 90.00° 91.21° 90.00°	Depositor
Resolution (Å)	28.87 – 3.58 28.86 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.87-3.58) 99.6 (28.86-3.58)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.55Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.284 , 0.313 0.288 , 0.316	Depositor DCC
$R_{free}$ test set	2461 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.9	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 99.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	94656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.26	0/5186	0.49	0/7037
1	3	0.26	0/5186	0.48	0/7037
1	5	0.26	0/5186	0.48	0/7037
1	A	0.26	0/5186	0.49	0/7037
1	C	0.26	0/5186	0.49	0/7037
1	E	0.26	0/5186	0.49	0/7037
1	G	0.26	0/5186	0.48	0/7037
1	I	0.26	0/5186	0.49	0/7037
1	K	0.26	0/5186	0.49	0/7037
1	M	0.26	0/5186	0.49	0/7037
1	O	0.26	0/5186	0.49	0/7037
1	Q	0.26	0/5186	0.49	0/7037
1	S	0.26	0/5186	0.49	0/7037
1	U	0.26	0/5186	0.49	0/7037
1	W	0.26	0/5186	0.50	0/7037
1	Y	0.26	0/5186	0.49	0/7037
2	2	0.27	0/853	0.51	0/1157
2	4	0.27	0/853	0.52	0/1157
2	6	0.27	0/853	0.51	0/1157
2	B	0.27	0/853	0.55	0/1157
2	D	0.27	0/853	0.52	0/1157
2	F	0.28	0/853	0.51	0/1157
2	H	0.27	0/853	0.53	0/1157
2	J	0.27	0/853	0.54	0/1157
2	L	0.27	0/853	0.56	0/1157
2	N	0.27	0/853	0.52	0/1157
2	P	0.26	0/853	0.53	0/1157
2	R	0.26	0/853	0.51	0/1157
2	T	0.27	0/853	0.54	0/1157
2	V	0.27	0/853	0.54	0/1157
2	X	0.27	0/853	0.55	0/1157
2	Z	0.27	0/853	0.54	0/1157
All	All	0.26	0/96624	0.49	0/131104

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	1	5078	0	5095	265	0
1	3	5078	0	5095	233	0
1	5	5078	0	5095	240	0
1	A	5078	0	5095	245	0
1	C	5078	0	5095	257	0
1	E	5078	0	5095	242	0
1	G	5078	0	5095	253	0
1	I	5078	0	5095	265	0
1	K	5078	0	5095	237	0
1	M	5078	0	5095	257	0
1	O	5078	0	5095	251	0
1	Q	5078	0	5095	240	0
1	S	5078	0	5095	252	0
1	U	5078	0	5095	250	0
1	W	5078	0	5095	241	0
1	Y	5078	0	5095	237	0
2	2	838	0	826	50	0
2	4	838	0	826	54	0
2	6	838	0	826	68	0
2	B	838	0	826	55	0
2	D	838	0	826	63	0
2	F	838	0	826	49	0
2	H	838	0	826	51	0
2	J	838	0	826	62	0
2	L	838	0	826	50	0
2	N	838	0	826	59	0
2	P	838	0	826	58	0
2	R	838	0	826	46	0
2	T	838	0	826	63	0
2	V	838	0	826	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	838	0	826	52	0
2	Z	838	0	826	48	0
All	All	94656	0	94736	4586	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 4586 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:456:ALA:H	1:5:630:THR:HG22	1.16	1.09
1:O:60:ASN:HB3	1:O:63:GLU:HB2	1.39	1.05
1:E:60:ASN:HB3	1:E:63:GLU:HB2	1.39	1.05
1:A:456:ALA:H	1:A:630:THR:HG22	1.21	1.05
1:O:456:ALA:H	1:O:630:THR:HG22	1.19	1.04

There are no symmetry-related clashes.

## 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	1	651/653 (100%)	549 (84%)	83 (13%)	19 (3%)	4	33
1	3	651/653 (100%)	556 (85%)	78 (12%)	17 (3%)	5	35
1	5	651/653 (100%)	552 (85%)	82 (13%)	17 (3%)	5	35
1	A	651/653 (100%)	545 (84%)	87 (13%)	19 (3%)	4	33
1	C	651/653 (100%)	550 (84%)	84 (13%)	17 (3%)	5	35
1	E	651/653 (100%)	551 (85%)	84 (13%)	16 (2%)	5	36
1	G	651/653 (100%)	555 (85%)	82 (13%)	14 (2%)	6	39
1	I	651/653 (100%)	551 (85%)	82 (13%)	18 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	651/653 (100%)	543 (83%)	87 (13%)	21 (3%)	4	31
1	M	651/653 (100%)	547 (84%)	83 (13%)	21 (3%)	4	31
1	O	651/653 (100%)	534 (82%)	93 (14%)	24 (4%)	3	28
1	Q	651/653 (100%)	545 (84%)	83 (13%)	23 (4%)	3	30
1	S	651/653 (100%)	549 (84%)	80 (12%)	22 (3%)	3	31
1	U	651/653 (100%)	543 (83%)	86 (13%)	22 (3%)	3	31
1	W	651/653 (100%)	551 (85%)	77 (12%)	23 (4%)	3	30
1	Y	651/653 (100%)	547 (84%)	86 (13%)	18 (3%)	5	34
2	2	106/108 (98%)	82 (77%)	16 (15%)	8 (8%)	1	12
2	4	106/108 (98%)	81 (76%)	18 (17%)	7 (7%)	1	16
2	6	106/108 (98%)	80 (76%)	18 (17%)	8 (8%)	1	12
2	B	106/108 (98%)	85 (80%)	14 (13%)	7 (7%)	1	16
2	D	106/108 (98%)	80 (76%)	15 (14%)	11 (10%)	0	7
2	F	106/108 (98%)	78 (74%)	20 (19%)	8 (8%)	1	12
2	H	106/108 (98%)	82 (77%)	17 (16%)	7 (7%)	1	16
2	J	106/108 (98%)	81 (76%)	17 (16%)	8 (8%)	1	12
2	L	106/108 (98%)	82 (77%)	17 (16%)	7 (7%)	1	16
2	N	106/108 (98%)	83 (78%)	16 (15%)	7 (7%)	1	16
2	P	106/108 (98%)	85 (80%)	13 (12%)	8 (8%)	1	12
2	R	106/108 (98%)	84 (79%)	15 (14%)	7 (7%)	1	16
2	T	106/108 (98%)	82 (77%)	16 (15%)	8 (8%)	1	12
2	V	106/108 (98%)	81 (76%)	15 (14%)	10 (9%)	0	9
2	X	106/108 (98%)	82 (77%)	15 (14%)	9 (8%)	1	10
2	Z	106/108 (98%)	83 (78%)	15 (14%)	8 (8%)	1	12
All	All	12112/12176 (100%)	10079 (83%)	1594 (13%)	439 (4%)	3	29

5 of 439 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	97	GLU
2	B	25	ALA
1	C	97	GLU
2	D	25	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1	559/559 (100%)	528 (94%)	31 (6%)	21	56
1	3	559/559 (100%)	528 (94%)	31 (6%)	21	56
1	5	559/559 (100%)	532 (95%)	27 (5%)	25	60
1	A	559/559 (100%)	522 (93%)	37 (7%)	16	51
1	C	559/559 (100%)	522 (93%)	37 (7%)	16	51
1	E	559/559 (100%)	530 (95%)	29 (5%)	23	58
1	G	559/559 (100%)	531 (95%)	28 (5%)	24	59
1	I	559/559 (100%)	529 (95%)	30 (5%)	22	57
1	K	559/559 (100%)	532 (95%)	27 (5%)	25	60
1	M	559/559 (100%)	534 (96%)	25 (4%)	27	62
1	O	559/559 (100%)	527 (94%)	32 (6%)	20	55
1	Q	559/559 (100%)	525 (94%)	34 (6%)	18	53
1	S	559/559 (100%)	528 (94%)	31 (6%)	21	56
1	U	559/559 (100%)	524 (94%)	35 (6%)	18	52
1	W	559/559 (100%)	526 (94%)	33 (6%)	19	54
1	Y	559/559 (100%)	533 (95%)	26 (5%)	26	61
2	2	95/95 (100%)	84 (88%)	11 (12%)	5	29
2	4	95/95 (100%)	87 (92%)	8 (8%)	11	42
2	6	95/95 (100%)	85 (90%)	10 (10%)	7	33
2	B	95/95 (100%)	87 (92%)	8 (8%)	11	42
2	D	95/95 (100%)	86 (90%)	9 (10%)	8	37
2	F	95/95 (100%)	85 (90%)	10 (10%)	7	33
2	H	95/95 (100%)	88 (93%)	7 (7%)	13	46
2	J	95/95 (100%)	84 (88%)	11 (12%)	5	29
2	L	95/95 (100%)	85 (90%)	10 (10%)	7	33
2	N	95/95 (100%)	85 (90%)	10 (10%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	95/95 (100%)	83 (87%)	12 (13%)	4	24
2	R	95/95 (100%)	85 (90%)	10 (10%)	7	33
2	T	95/95 (100%)	84 (88%)	11 (12%)	5	29
2	V	95/95 (100%)	86 (90%)	9 (10%)	8	37
2	X	95/95 (100%)	85 (90%)	10 (10%)	7	33
2	Z	95/95 (100%)	85 (90%)	10 (10%)	7	33
All	All	10464/10464 (100%)	9815 (94%)	649 (6%)	18	53

5 of 649 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	212	SER
2	R	113	THR
1	3	494	MET
1	O	483	ARG
1	Q	77	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 250 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	366	HIS
2	R	73	GLN
2	4	73	GLN
1	O	439	GLN
1	Q	116	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	1	653/653 (100%)	-0.38	1 (0%) 95 91	68, 113, 161, 218	0
1	3	653/653 (100%)	-0.06	14 (2%) 63 46	76, 118, 187, 244	0
1	5	653/653 (100%)	-0.04	12 (1%) 68 51	74, 118, 182, 243	0
1	A	653/653 (100%)	-0.36	4 (0%) 89 80	70, 115, 162, 220	0
1	C	653/653 (100%)	-0.30	0 100 100	53, 108, 157, 205	0
1	E	653/653 (100%)	-0.37	4 (0%) 89 80	68, 111, 161, 206	0
1	G	653/653 (100%)	-0.37	5 (0%) 86 73	68, 113, 162, 214	0
1	I	653/653 (100%)	-0.42	1 (0%) 95 91	66, 112, 161, 220	0
1	K	653/653 (100%)	-0.36	4 (0%) 89 80	63, 109, 161, 225	0
1	M	653/653 (100%)	-0.40	3 (0%) 91 82	56, 110, 158, 209	0
1	O	653/653 (100%)	-0.33	1 (0%) 95 91	59, 109, 159, 224	0
1	Q	653/653 (100%)	-0.41	5 (0%) 86 73	69, 114, 162, 211	0
1	S	653/653 (100%)	-0.35	2 (0%) 94 88	63, 109, 157, 217	0
1	U	653/653 (100%)	-0.39	2 (0%) 94 88	70, 114, 161, 224	0
1	W	653/653 (100%)	-0.30	7 (1%) 80 66	69, 115, 161, 206	0
1	Y	653/653 (100%)	-0.26	7 (1%) 80 66	71, 116, 165, 235	0
2	2	108/108 (100%)	0.17	9 (8%) 11 6	83, 127, 206, 241	0
2	4	108/108 (100%)	0.80	18 (16%) 1 0	94, 152, 229, 249	0
2	6	108/108 (100%)	0.78	19 (17%) 1 0	91, 151, 229, 279	0
2	B	108/108 (100%)	0.25	12 (11%) 5 3	89, 137, 214, 260	0
2	D	108/108 (100%)	0.02	4 (3%) 41 25	78, 119, 204, 240	0
2	F	108/108 (100%)	0.39	10 (9%) 8 4	89, 138, 216, 289	0
2	H	108/108 (100%)	0.09	10 (9%) 8 4	92, 135, 214, 242	0
2	J	108/108 (100%)	0.38	11 (10%) 6 3	81, 130, 214, 262	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	L	108/108 (100%)	0.21	11 (10%) 6 3	88, 132, 208, 248	0
2	N	108/108 (100%)	-0.05	4 (3%) 41 25	78, 120, 196, 240	0
2	P	108/108 (100%)	0.21	8 (7%) 14 8	83, 123, 214, 246	0
2	R	108/108 (100%)	0.28	13 (12%) 4 3	86, 138, 211, 253	0
2	T	108/108 (100%)	-0.03	4 (3%) 41 25	79, 123, 204, 240	0
2	V	108/108 (100%)	0.24	11 (10%) 6 3	90, 139, 220, 250	0
2	X	108/108 (100%)	0.23	13 (12%) 4 3	90, 133, 208, 250	0
2	Z	108/108 (100%)	0.21	15 (13%) 2 2	91, 142, 230, 251	0
All	All	12176/12176 (100%)	-0.24	244 (2%) 65 48	53, 115, 174, 289	0

The worst 5 of 244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	25	ALA	16.6
2	F	25	ALA	16.1
2	6	25	ALA	13.0
2	V	25	ALA	8.1
2	B	25	ALA	7.7

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.