



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:22 PM GMT

PDB ID : 4V4K  
Title : Bacteriophage P22 Portal Protein bound to middle Tail Factor GP4. This file  
contain the second biological assembly  
Authors : Olia, A.S.; Cingolani, G.  
Deposited on : 2010-04-19  
Resolution : 3.25 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



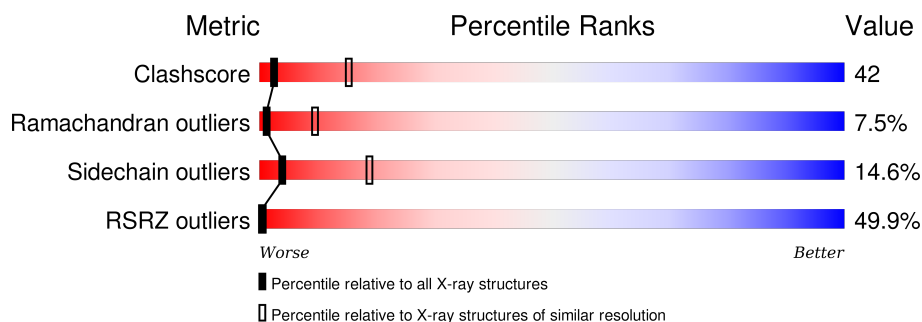
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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))
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	602	<div> <div>48%</div> <div> <div>38%</div> <div>44%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	602	<div> <div>52%</div> <div> <div>38%</div> <div>44%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	C	602	<div> <div>50%</div> <div> <div>37%</div> <div>45%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	D	602	<div> <div>44%</div> <div> <div>38%</div> <div>44%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	E	602	<div> <div>47%</div> <div> <div>38%</div> <div>45%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	F	602	<div> <div>44%</div> <div> <div>38%</div> <div>43%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	G	602	<div> <div>46%</div> <div> <div>38%</div> <div>44%</div> <div>12%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	602	
1	I	602	
1	J	602	
1	K	602	
1	L	602	
1	M	602	
1	N	602	
1	O	602	
1	P	602	
1	Q	602	
1	R	602	
1	S	602	
1	T	602	
1	U	602	
1	V	602	
1	W	602	
1	X	602	
2	Y	166	
2	Z	166	
2	a	166	
2	b	166	
2	c	166	
2	d	166	
2	e	166	
2	f	166	

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Mol	Chain	Length	Quality of chain
2	g	166	
2	h	166	
2	i	166	
2	j	166	
2	k	166	
2	l	166	
2	m	166	
2	n	166	
2	o	166	
2	p	166	
2	q	166	
2	r	166	
2	s	166	
2	t	166	
2	u	166	
2	v	166	



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 135120 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 PORTAL PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	M	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	N	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	O	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	P	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	Q	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	R	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	S	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	T	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	U	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	V	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	W	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	X	569	Total	C	N	O	S	Se	0	0	0
			4564	2871	786	887	4	16			
1	A	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	B	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	C	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	D	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	F	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	G	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	H	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	I	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	J	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	K	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			
1	L	569	Total	C	N	O	S	Se	0	0	0
			4553	2865	783	885	4	16			

- Molecule 2 is a protein called PACKAGED DNA STABILIZATION PROTEIN GP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	k	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	l	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	m	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	n	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	o	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	p	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	q	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	r	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	s	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	t	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	u	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	v	145	Total	C	N	O	S	0	0	0
			1052	654	182	211	5			
2	Y	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	Z	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	a	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	b	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	c	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	d	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	e	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	f	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	g	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	h	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	i	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			
2	j	146	Total	C	N	O	S	0	0	0
			1048	652	179	212	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
l	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
m	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
n	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
o	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
p	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
q	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
r	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
s	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
t	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
u	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
v	141	PRO	ALA	ENGINEERED MUTATION	UNP P26746
Y	150	PRO	ALA	ENGINEERED	UNP P26746

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	150	PRO	ALA	ENGINEERED	UNP P26746
a	150	PRO	ALA	ENGINEERED	UNP P26746
b	150	PRO	ALA	ENGINEERED	UNP P26746
c	150	PRO	ALA	ENGINEERED	UNP P26746
d	150	PRO	ALA	ENGINEERED	UNP P26746
e	150	PRO	ALA	ENGINEERED	UNP P26746
f	150	PRO	ALA	ENGINEERED	UNP P26746
g	150	PRO	ALA	ENGINEERED	UNP P26746
h	150	PRO	ALA	ENGINEERED	UNP P26746
i	150	PRO	ALA	ENGINEERED	UNP P26746
j	150	PRO	ALA	ENGINEERED	UNP P26746

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	21	Total O 21 21	0	0
3	N	21	Total O 21 21	0	0
3	O	21	Total O 21 21	0	0
3	P	21	Total O 21 21	0	0
3	Q	21	Total O 21 21	0	0
3	R	21	Total O 21 21	0	0
3	S	21	Total O 21 21	0	0
3	T	21	Total O 21 21	0	0
3	U	21	Total O 21 21	0	0
3	V	21	Total O 21 21	0	0
3	W	21	Total O 21 21	0	0
3	X	21	Total O 21 21	0	0
3	A	22	Total O 22 22	0	0
3	B	22	Total O 22 22	0	0

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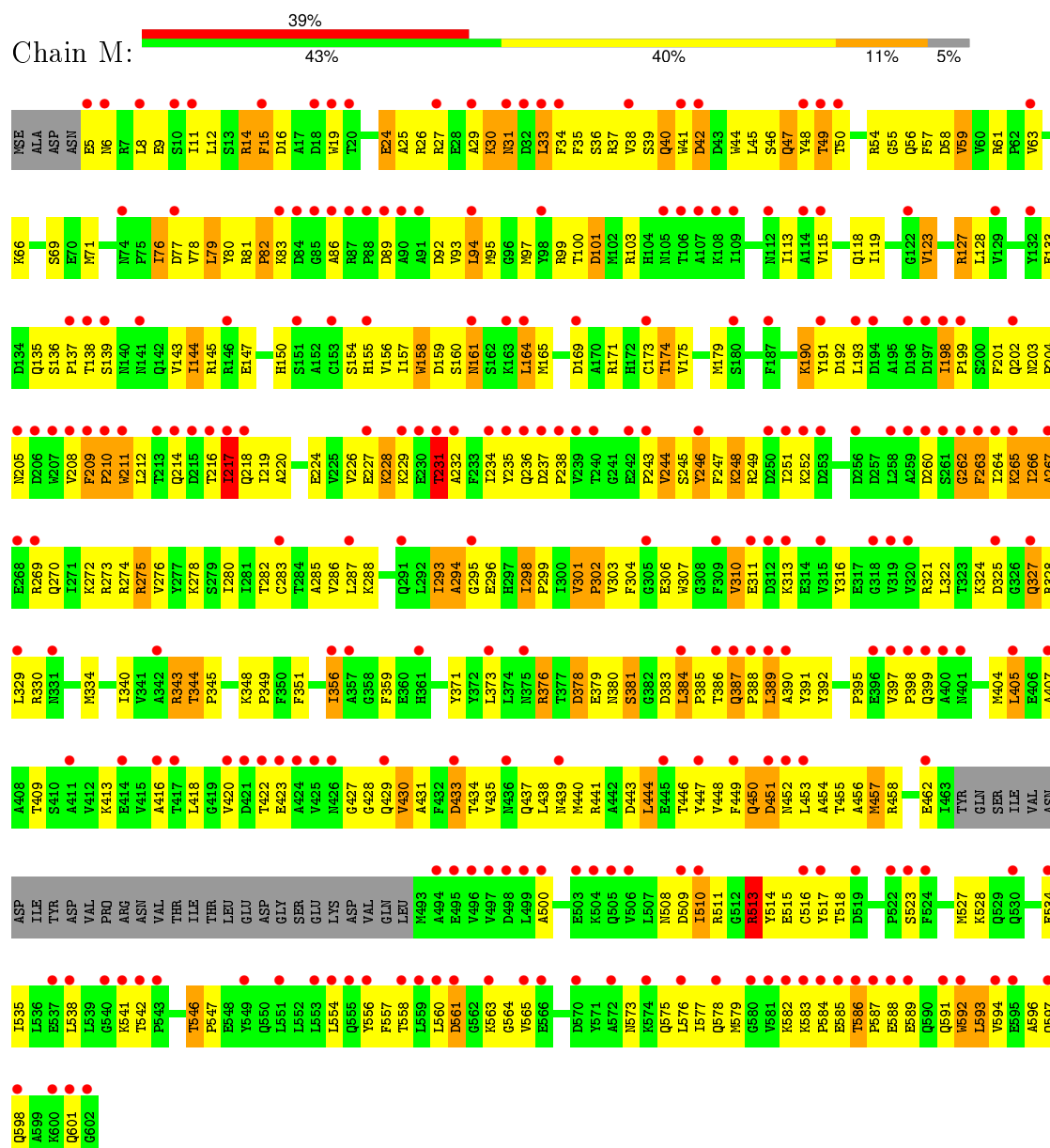
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	22	Total 22	O 22	0	0
3	D	22	Total 22	O 22	0	0
3	E	22	Total 22	O 22	0	0
3	F	22	Total 22	O 22	0	0
3	G	22	Total 22	O 22	0	0
3	H	22	Total 22	O 22	0	0
3	I	22	Total 22	O 22	0	0
3	J	22	Total 22	O 22	0	0
3	K	22	Total 22	O 22	0	0
3	L	22	Total 22	O 22	0	0



### 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 errors 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: PORTAL PROTEIN

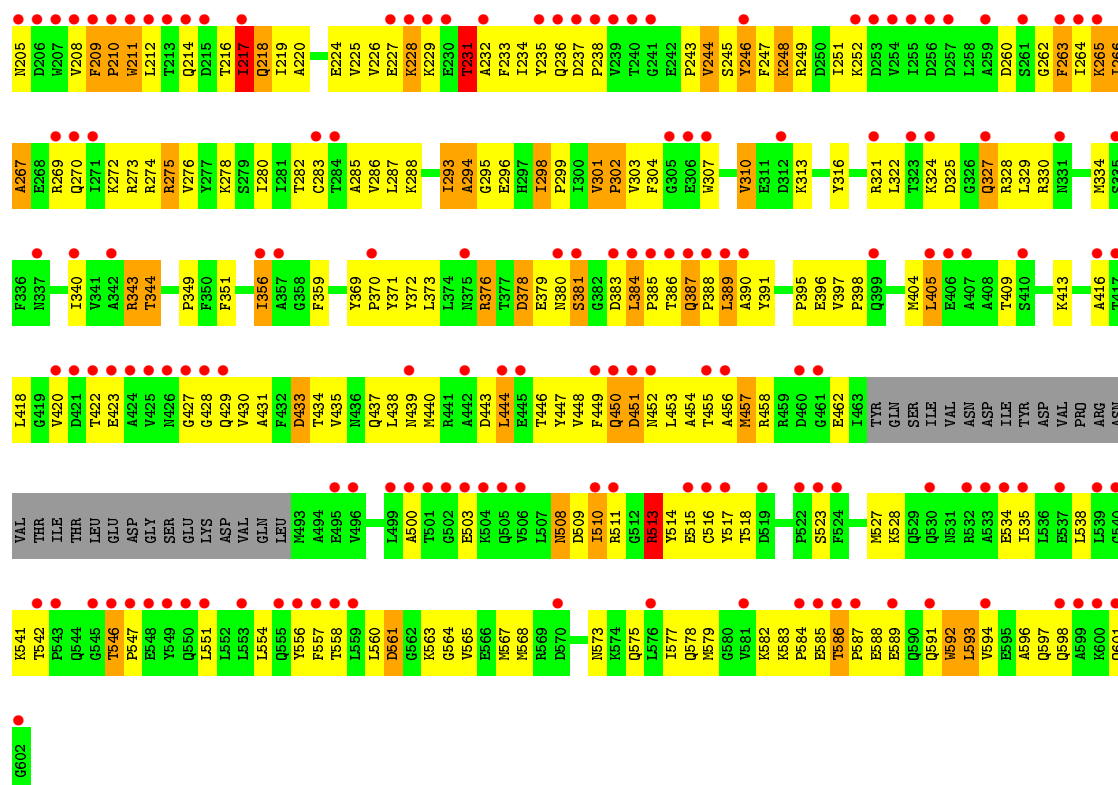


#### • Molecule 1: PORTAL PROTEIN

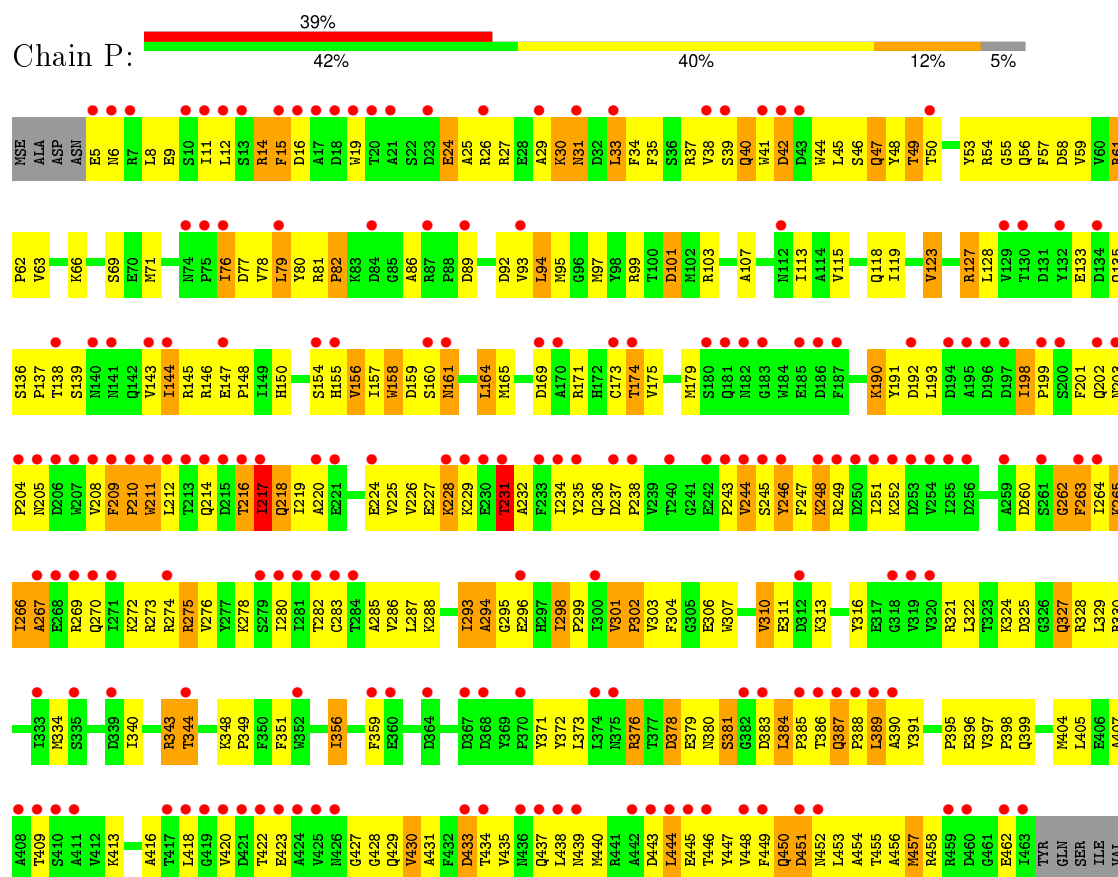




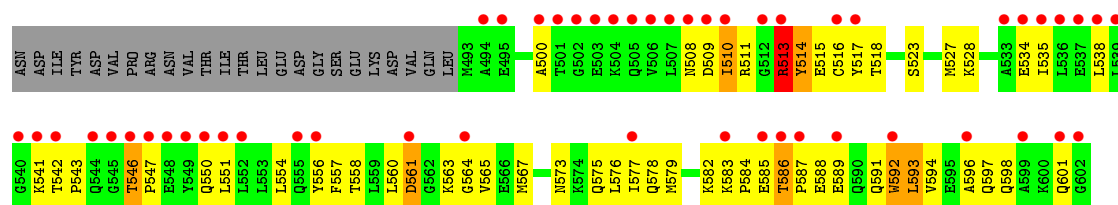




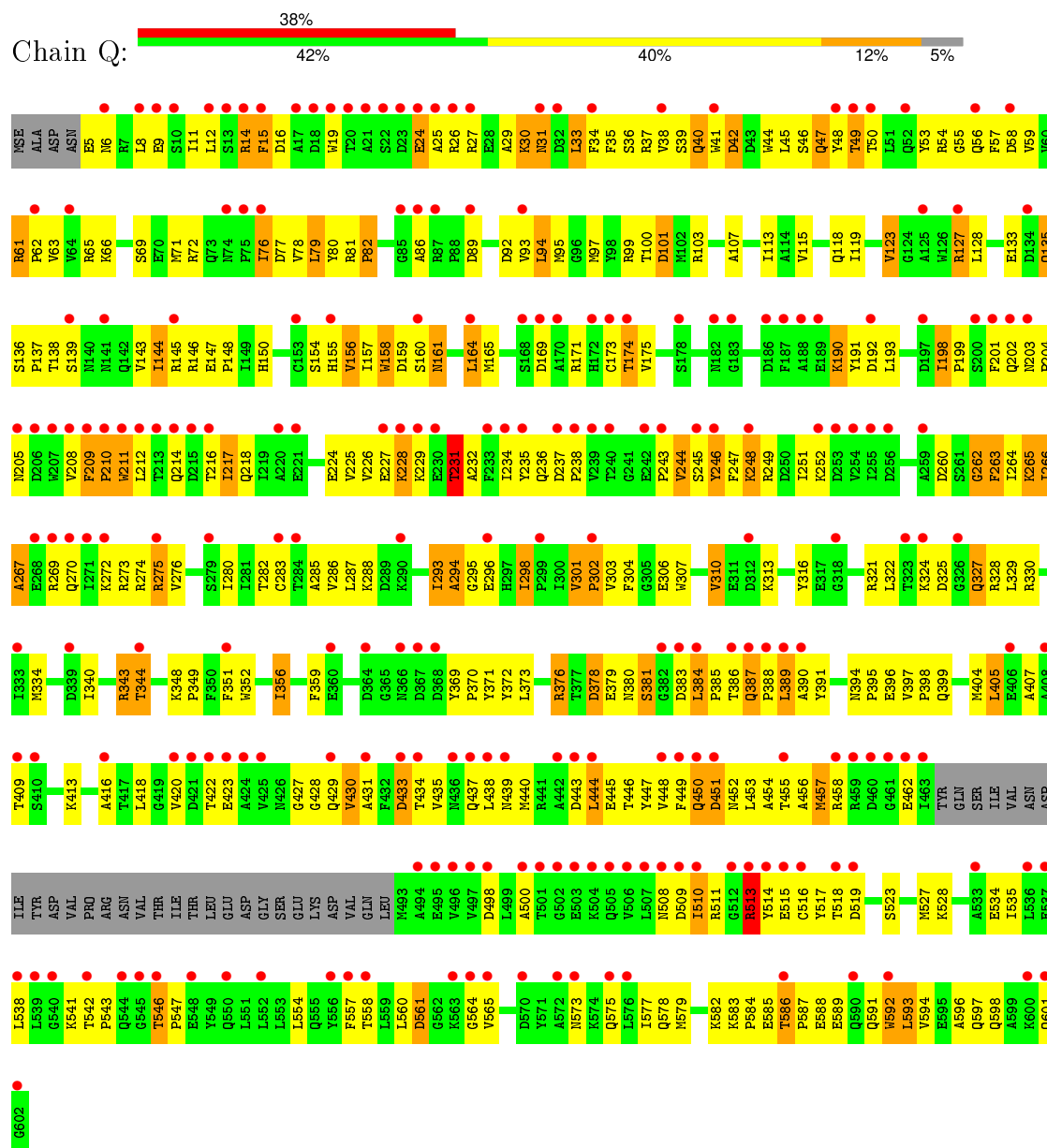
• Molecule 1: PORTAL PROTEIN



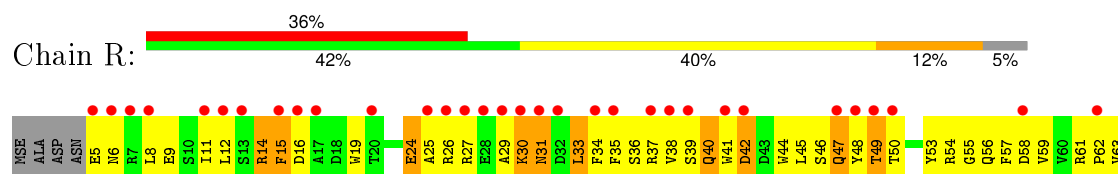




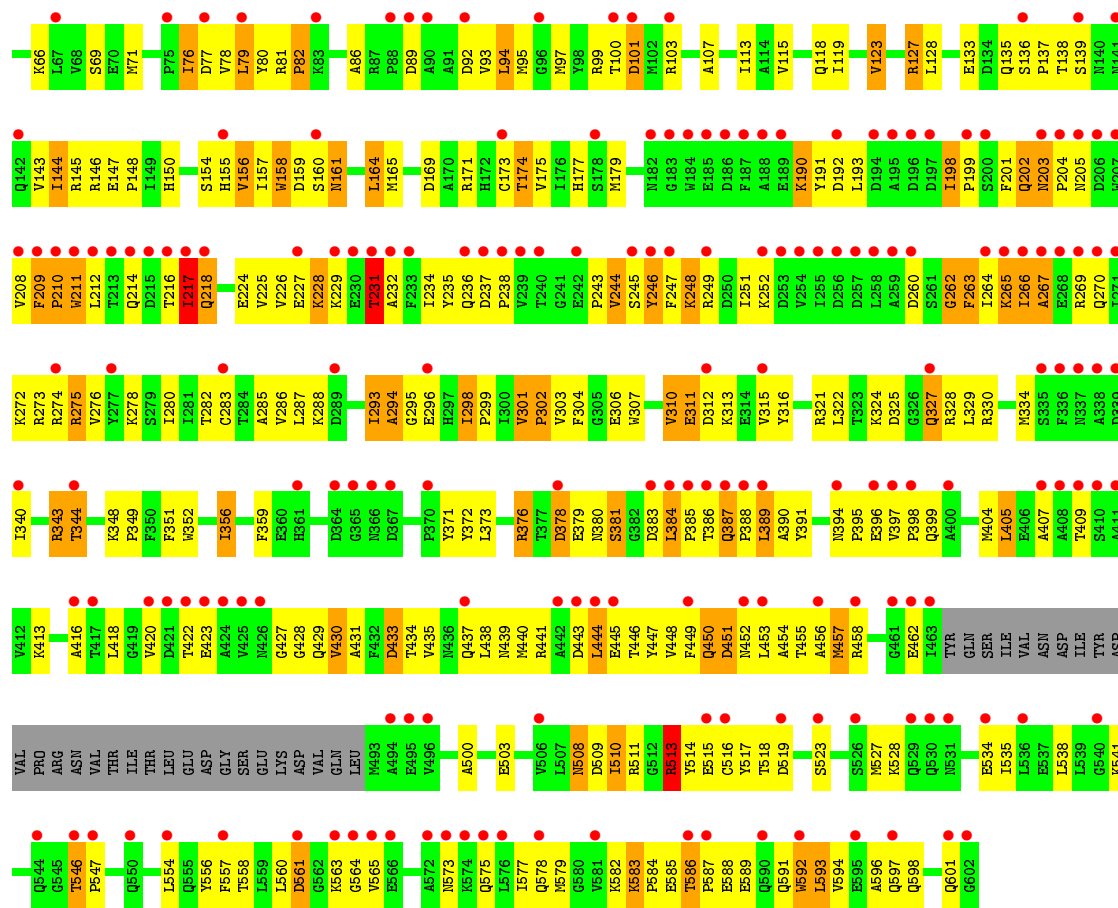
### • Molecule 1: PORTAL PROTEIN



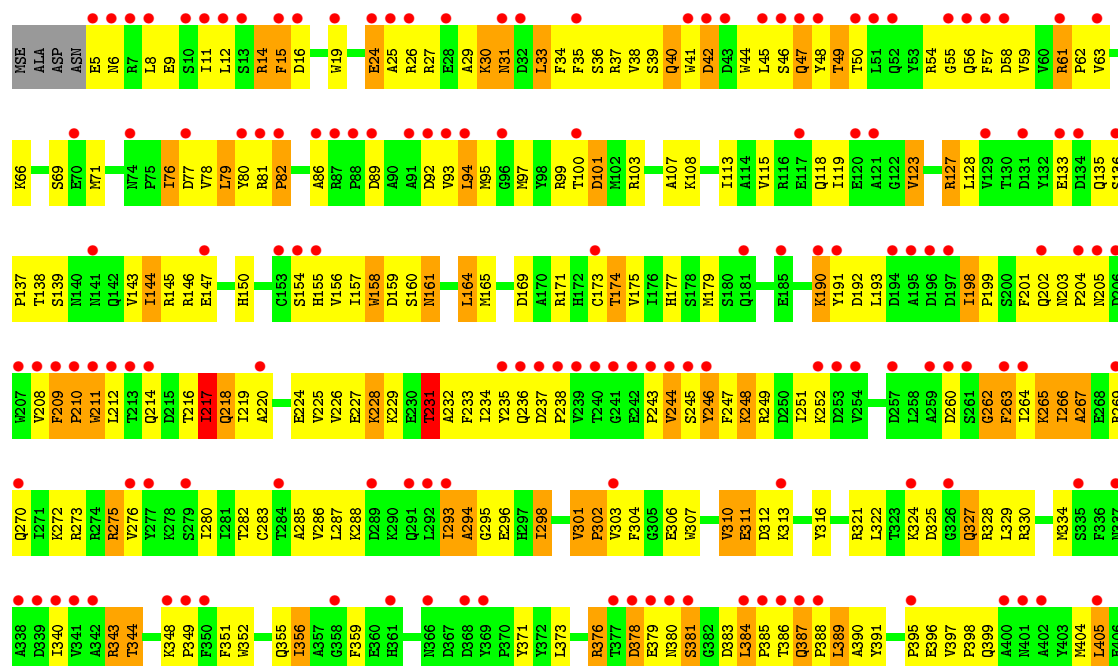
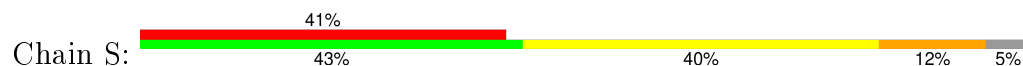
### • Molecule 1: PORTAL PROTEIN



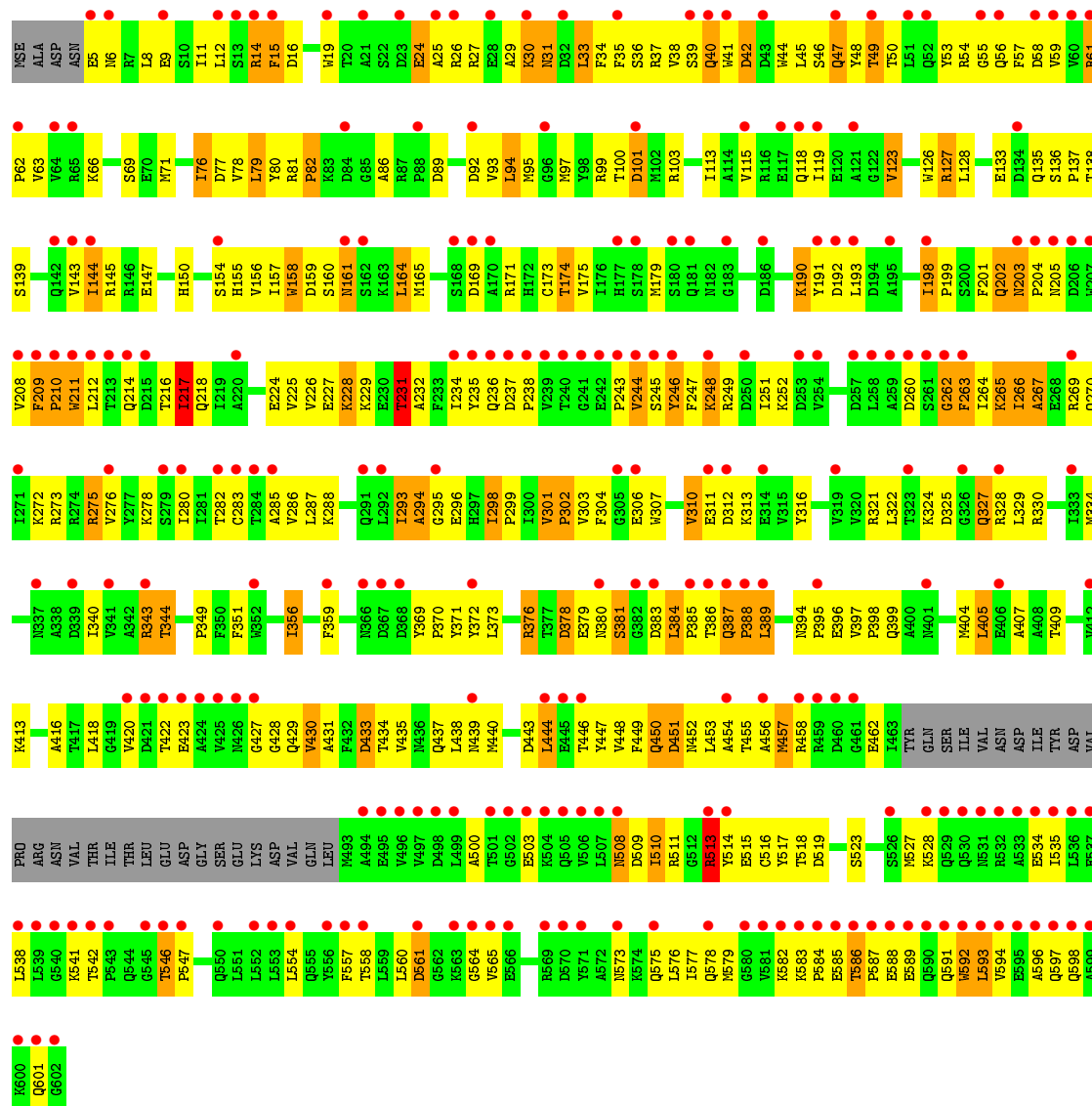




# Molecule 1: PORTAL PROTEIN

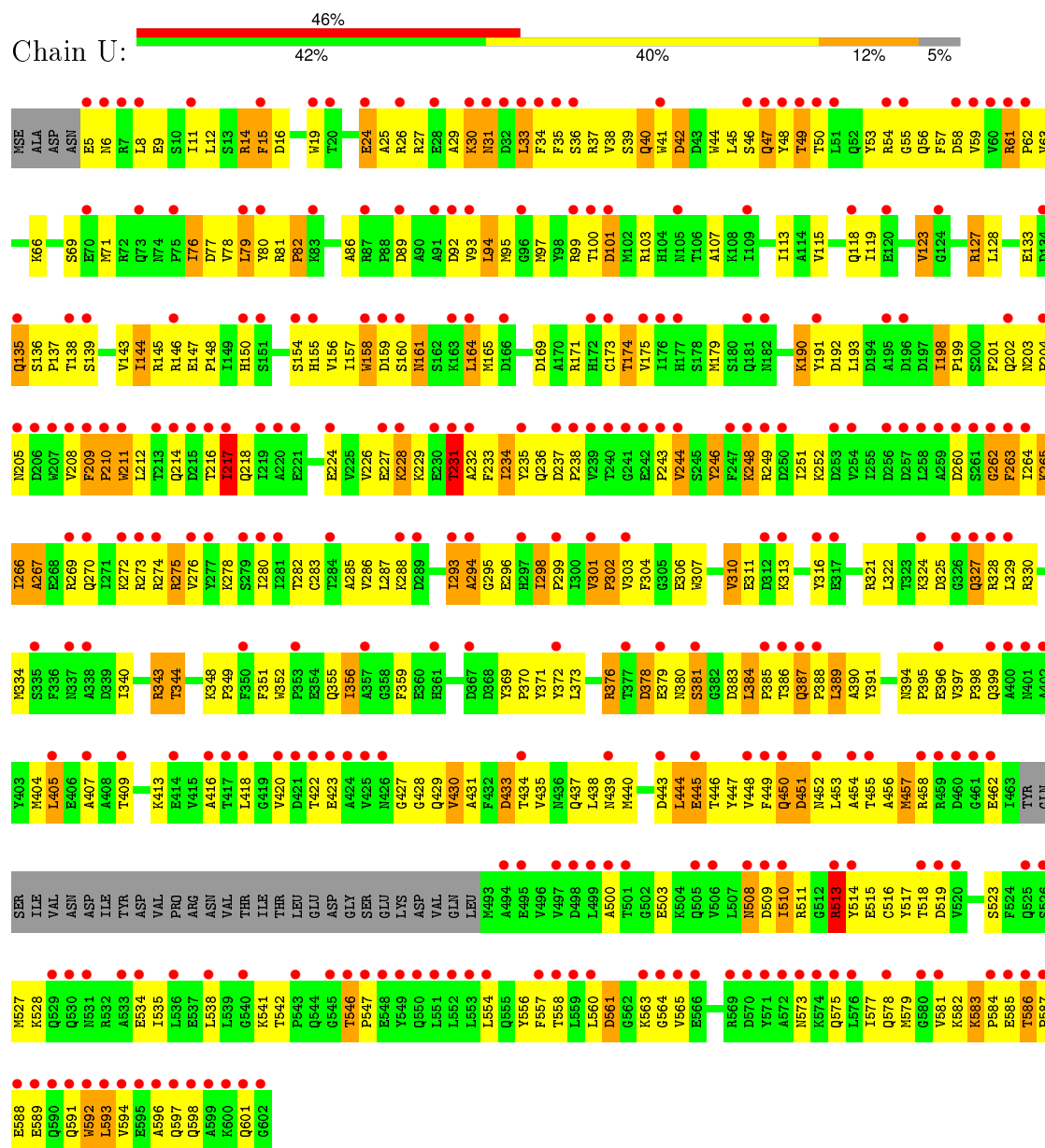




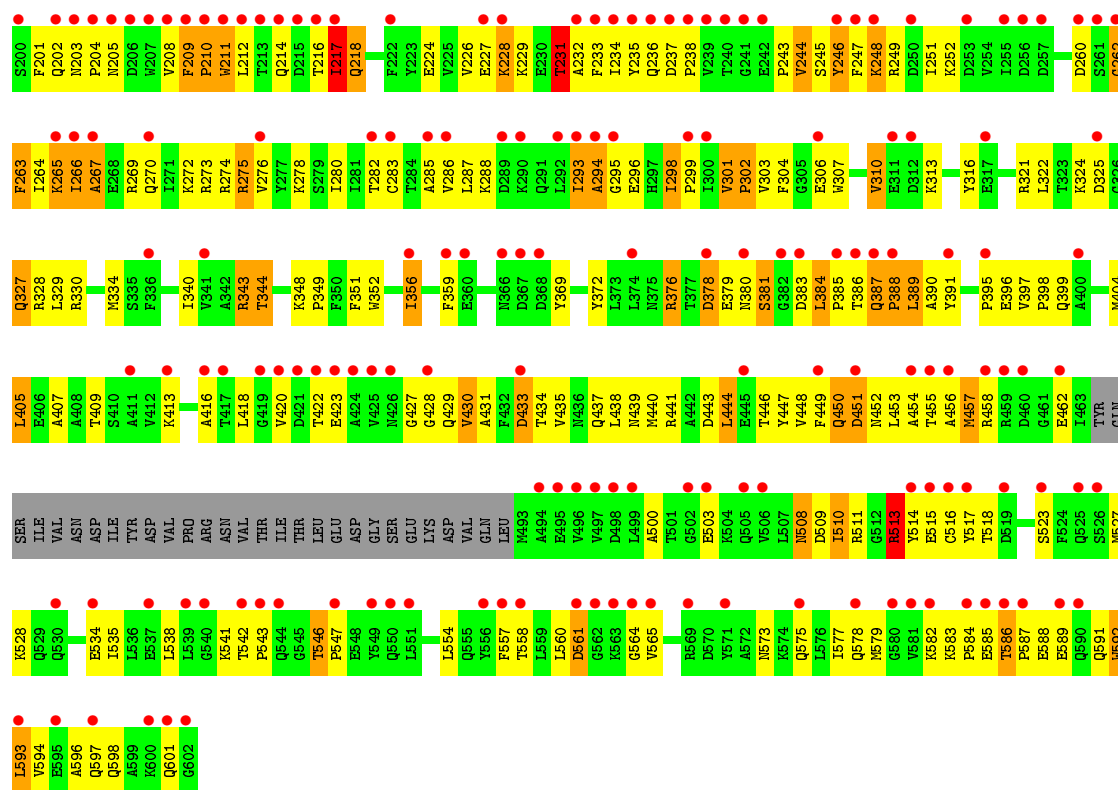




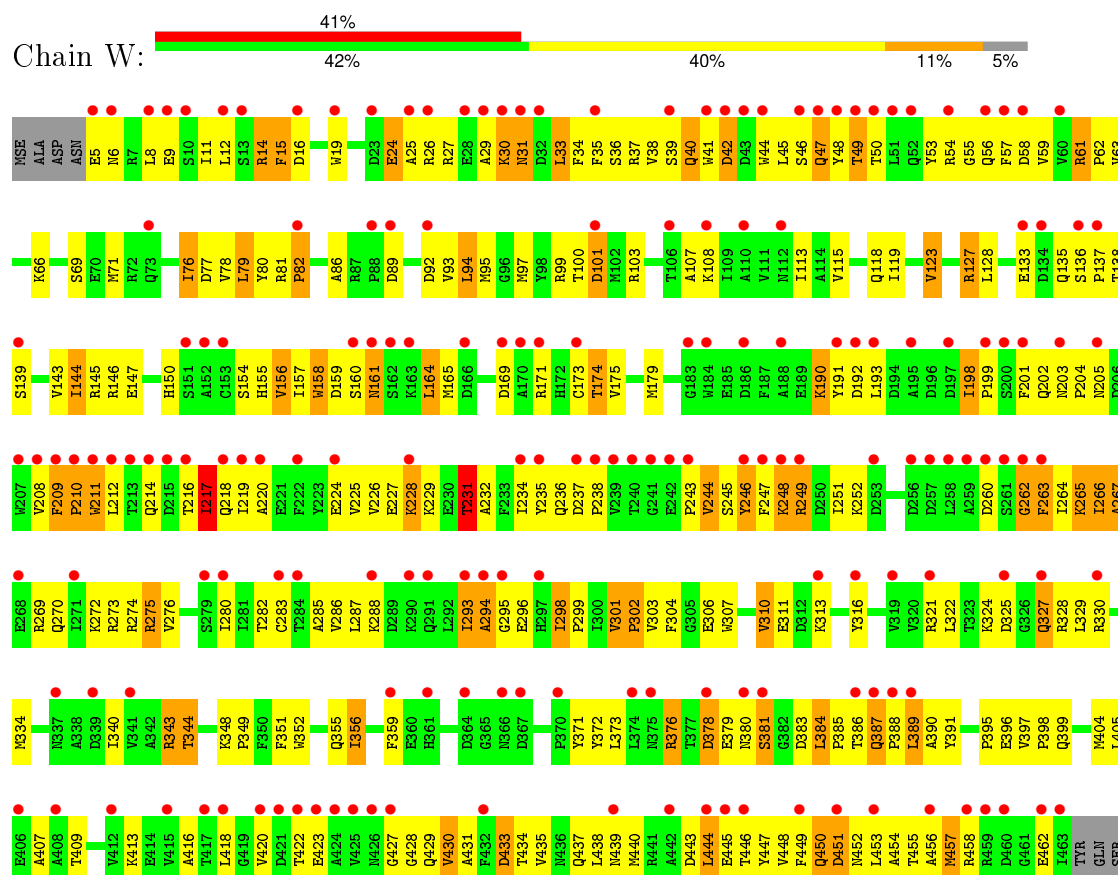
• Molecule 1: PORTAL PROTEIN



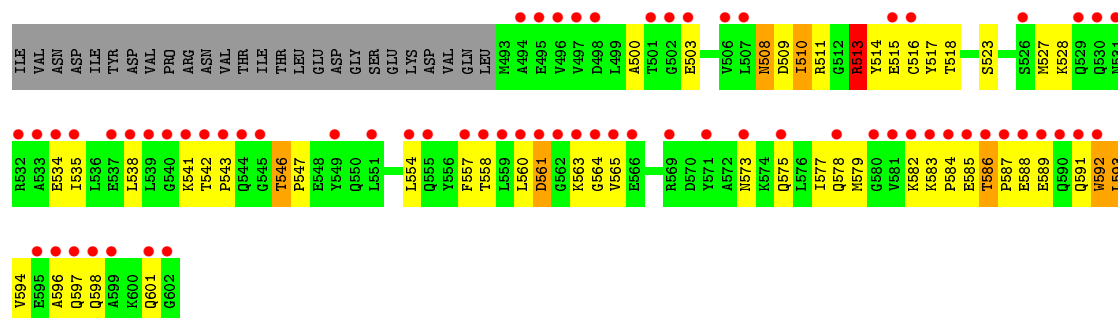




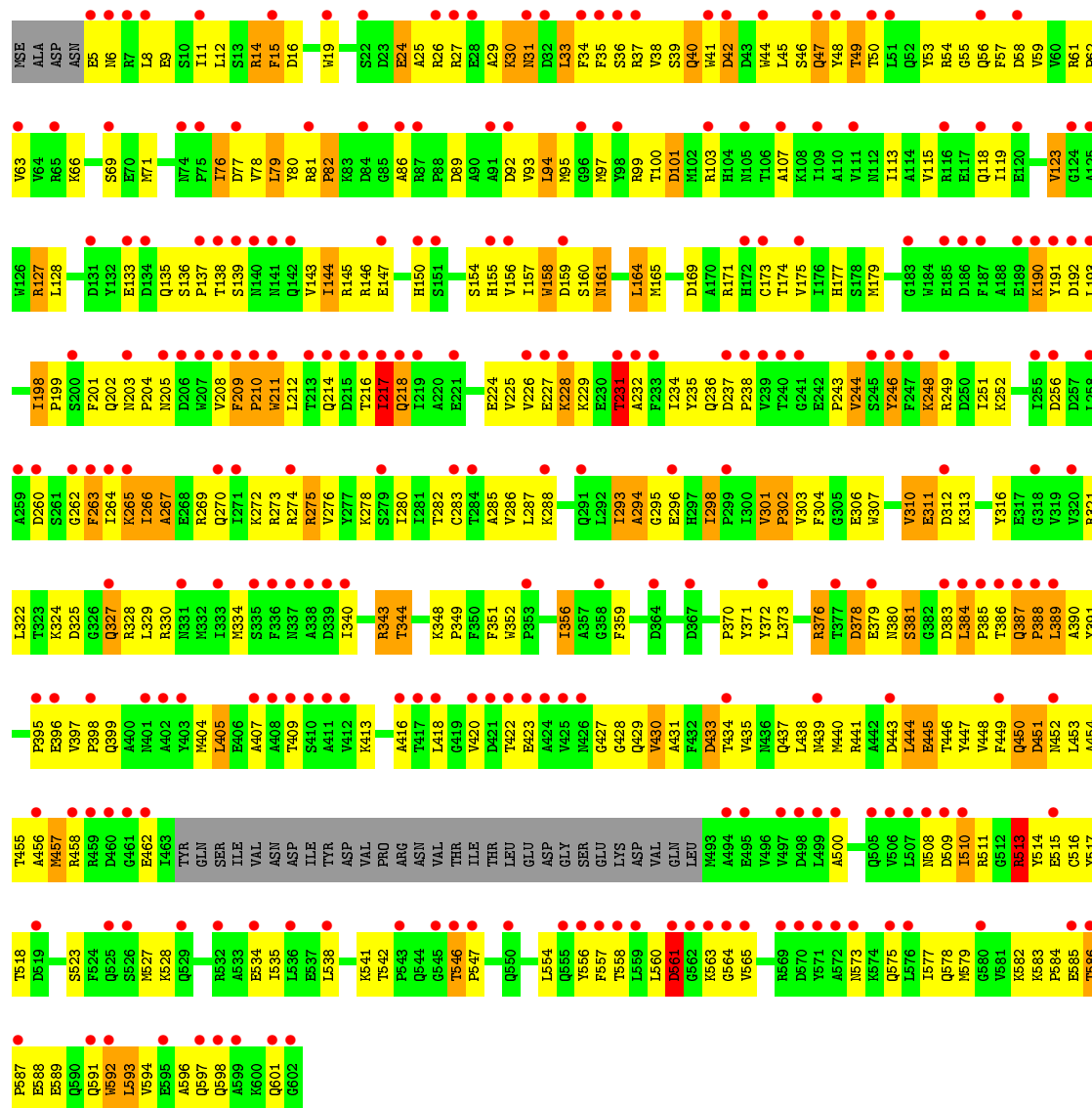
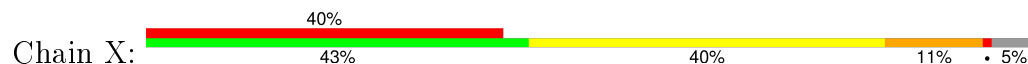
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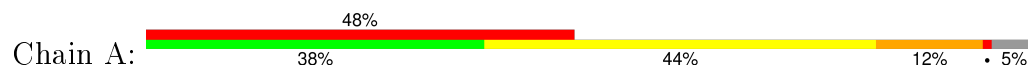




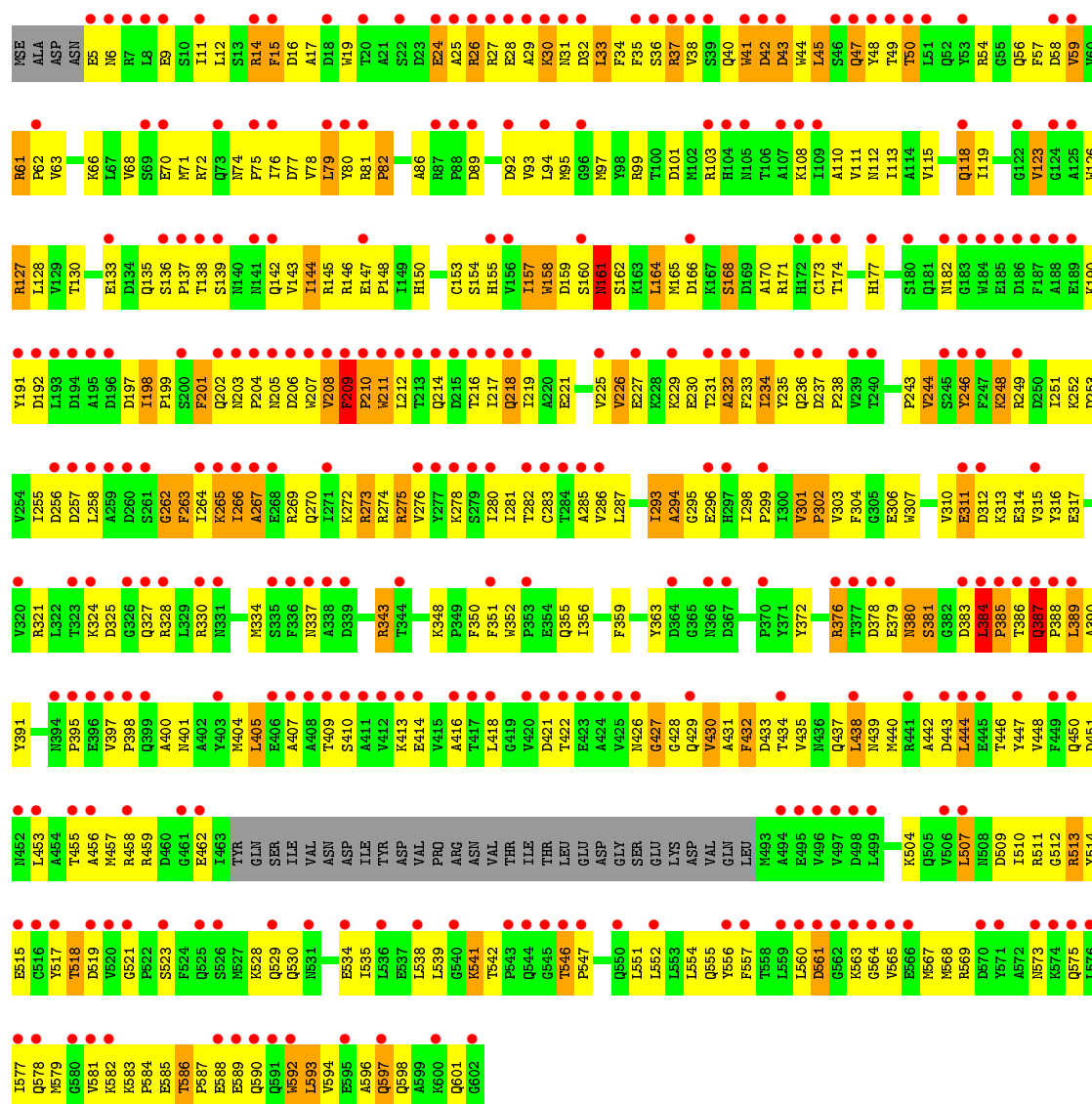
• Molecule 1: PORTAL PROTEIN



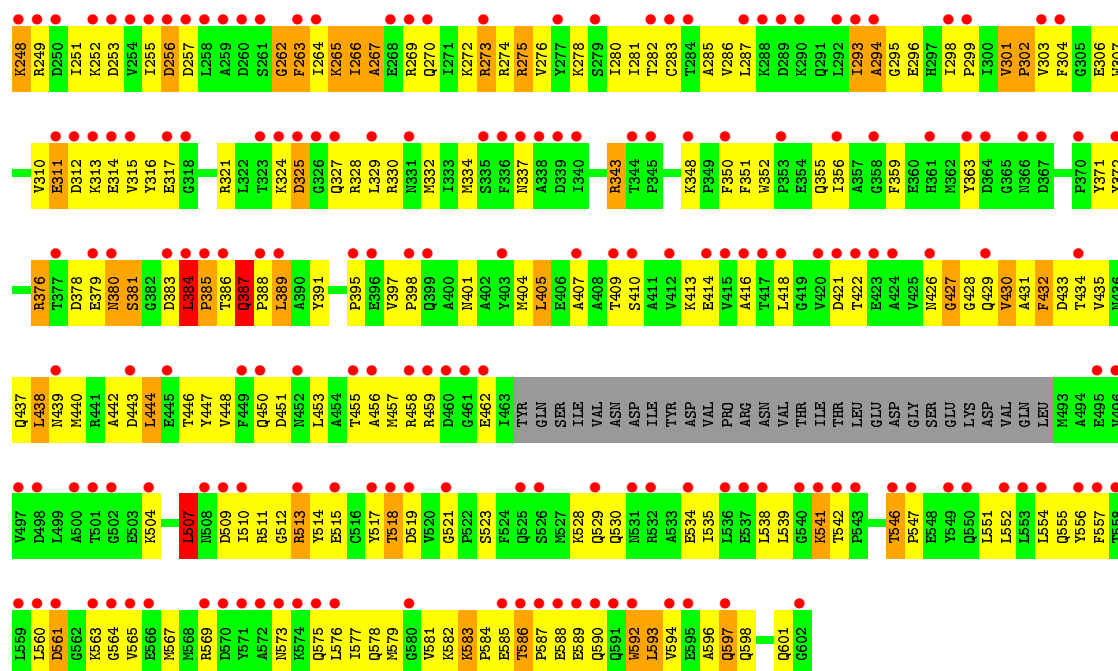
• Molecule 1: PORTAL PROTEIN



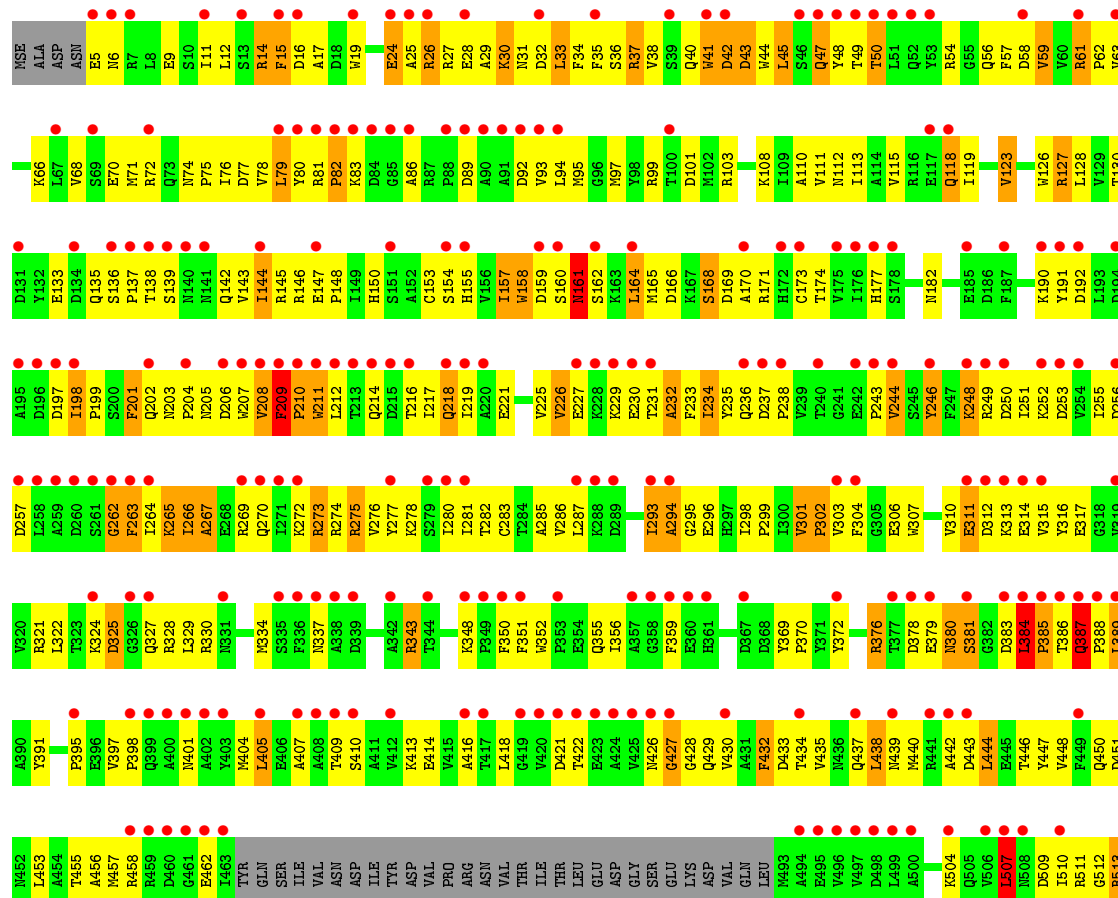




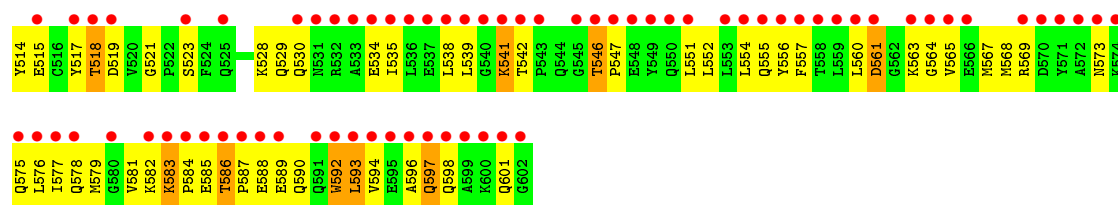




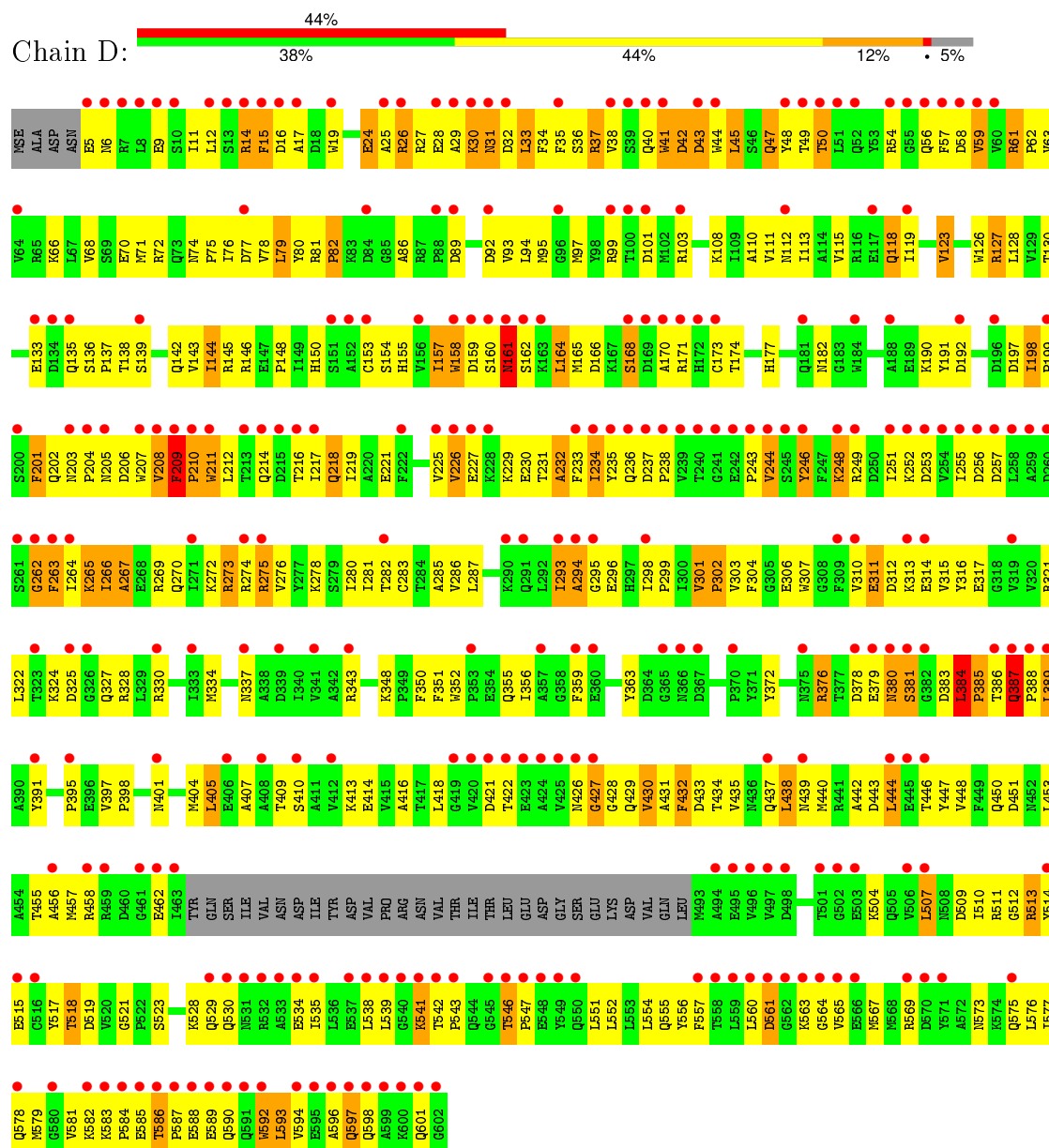
### • Molecule 1: PORTAL PROTEIN



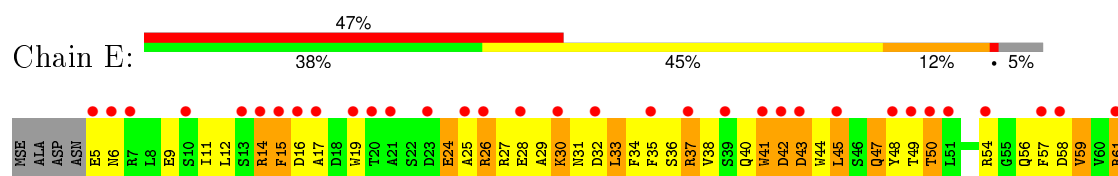




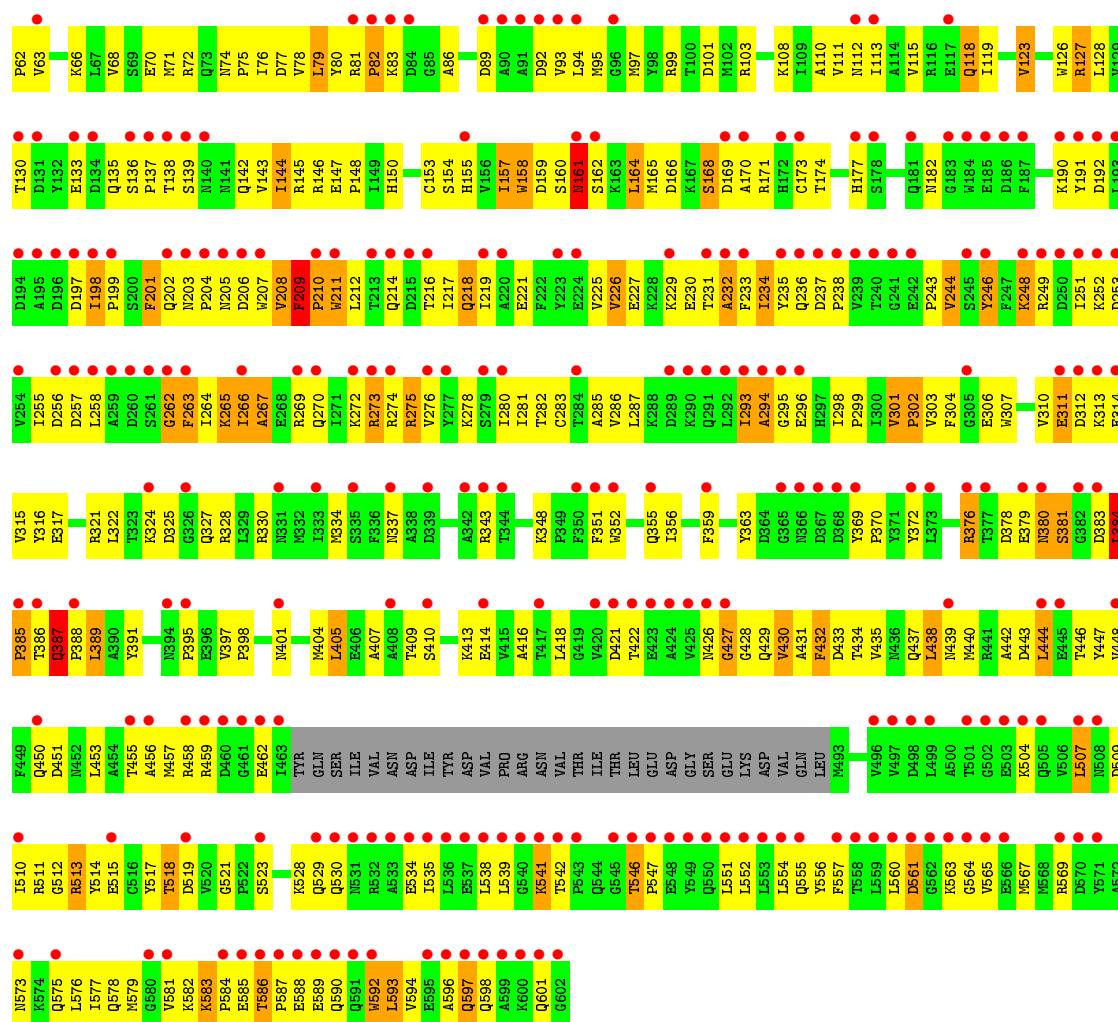
### • Molecule 1: PORTAL PROTEIN



### • Molecule 1: PORTAL PROTEIN

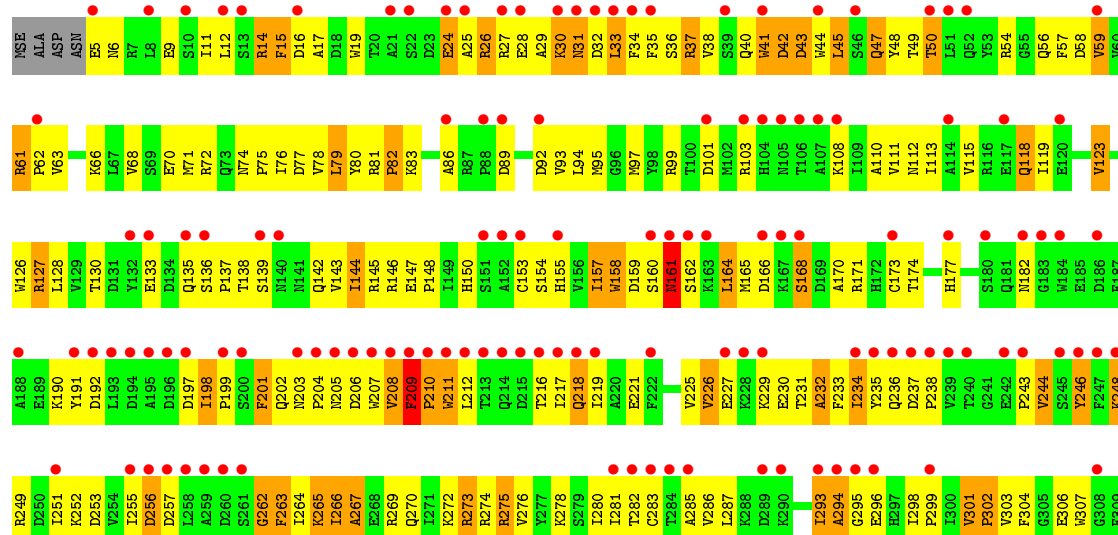




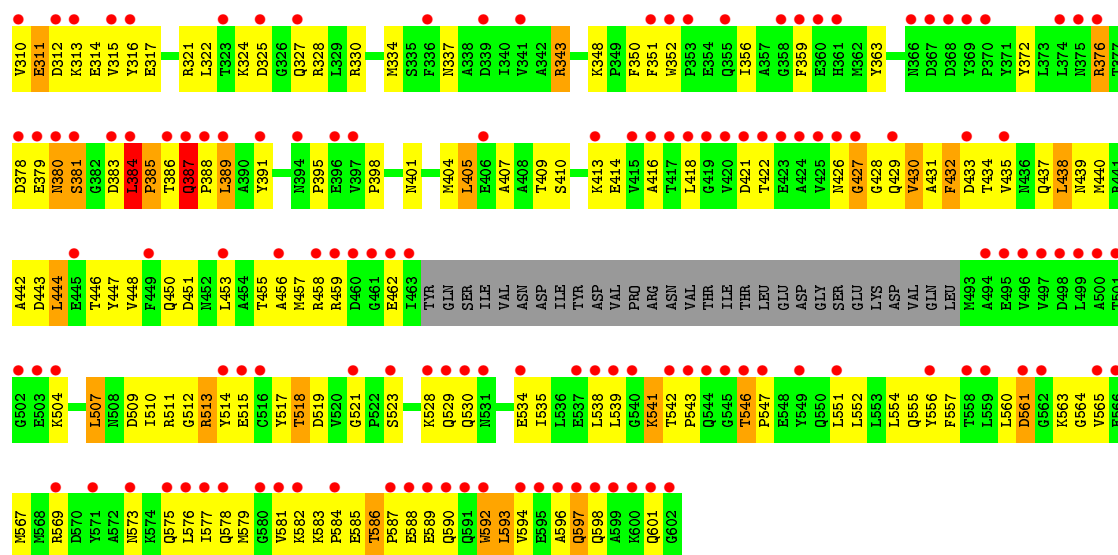


• Molecule 1: PORTAL PROTEIN

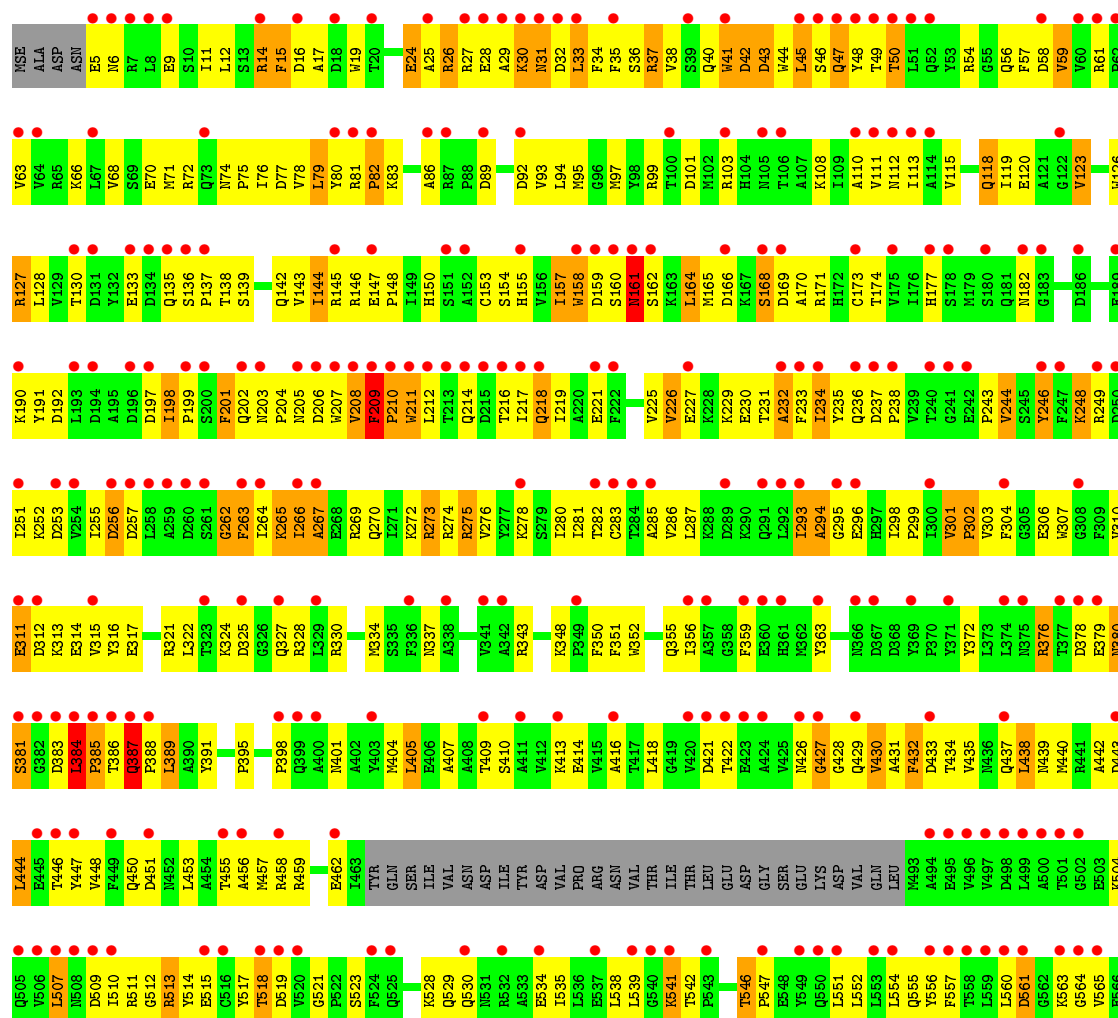
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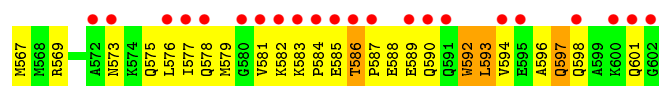




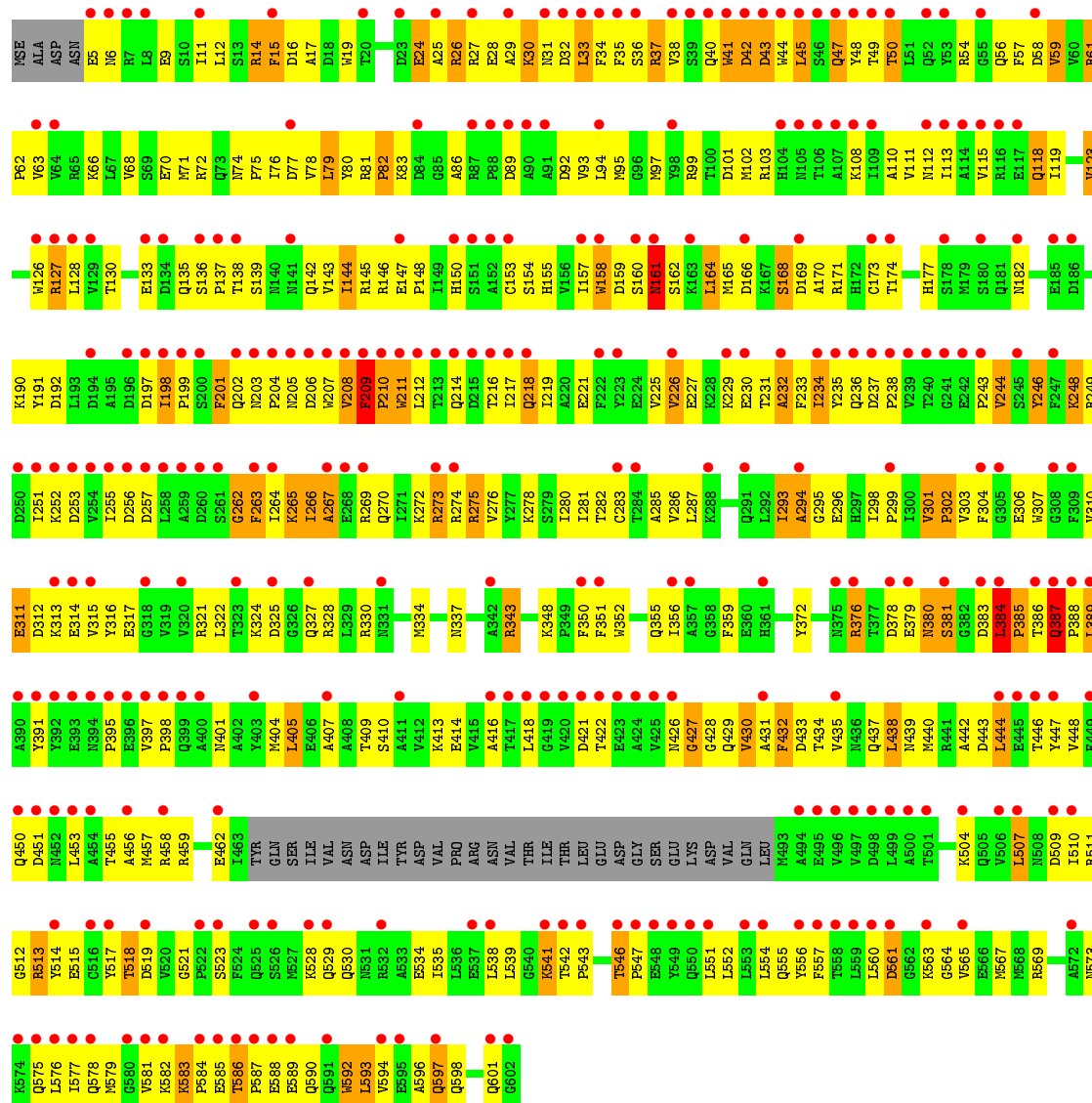
### • Molecule 1: PORTAL PROTEIN



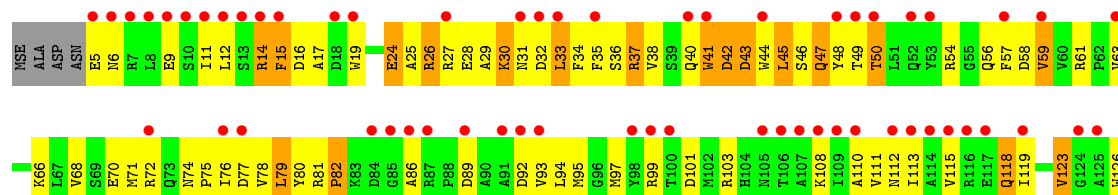




### • Molecule 1: PORTAL PROTEIN



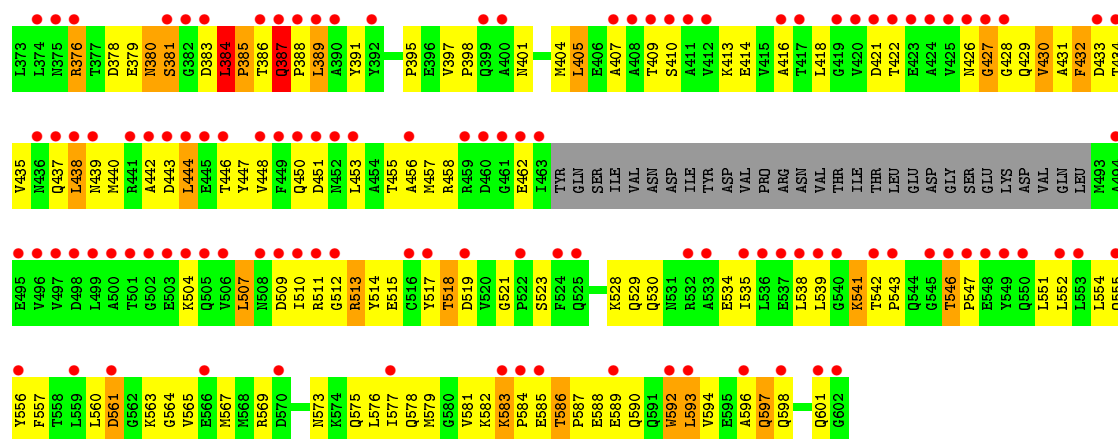
### • Molecule 1: PORTAL PROTEIN



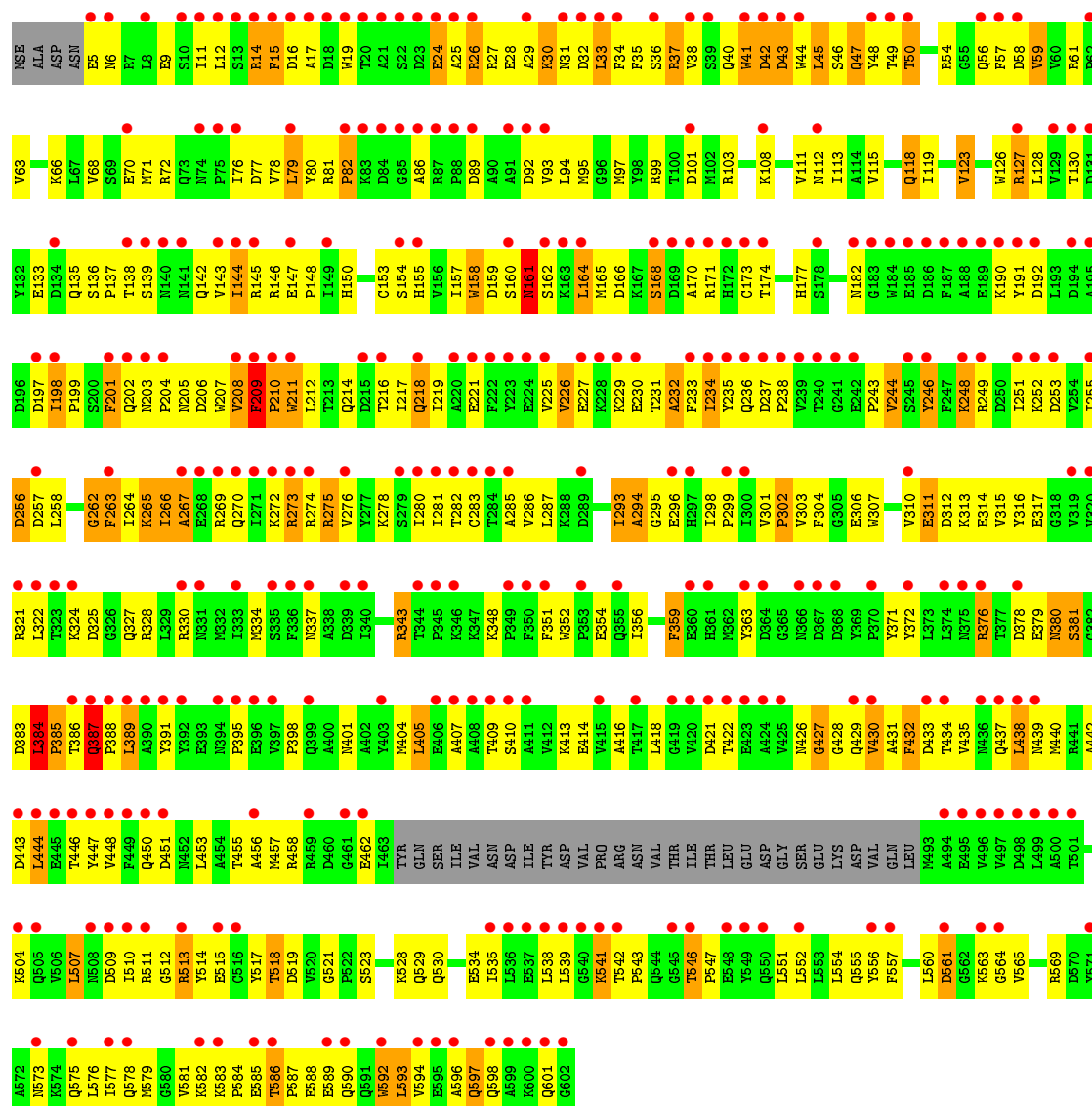








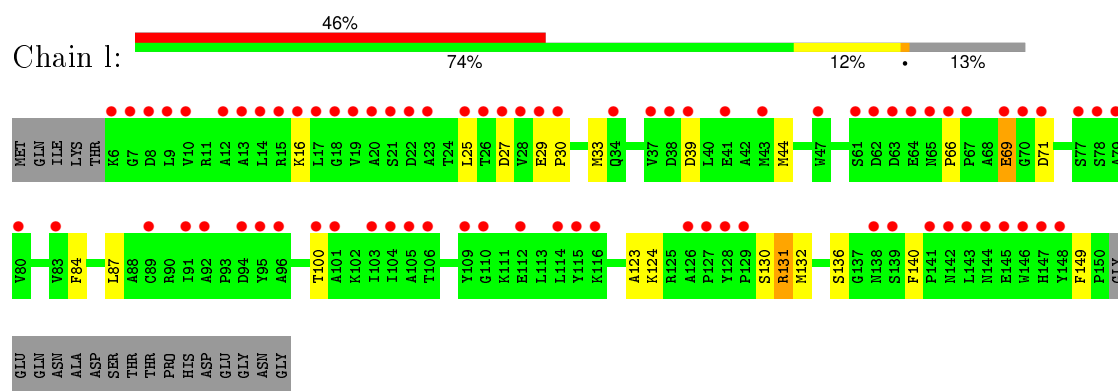
• Molecule 1: PORTAL PROTEIN



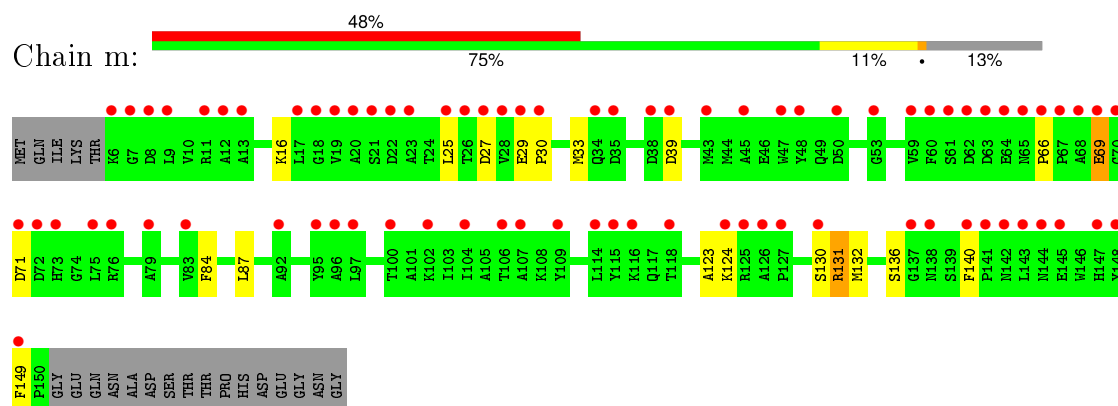




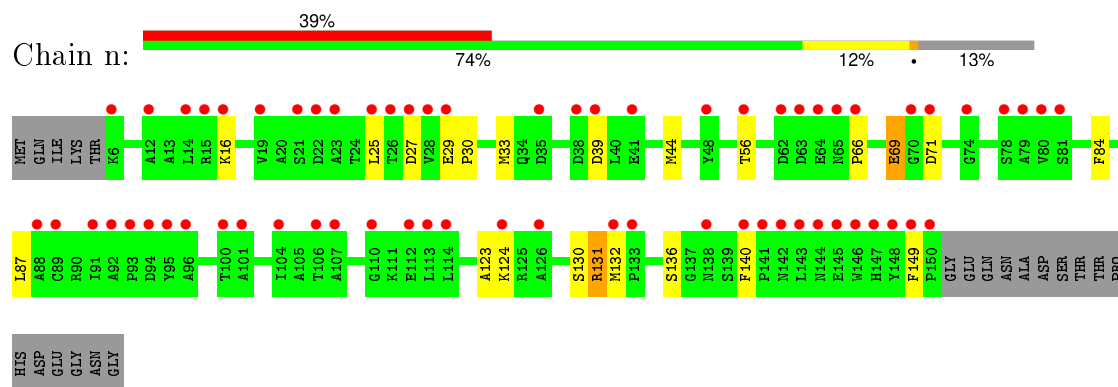




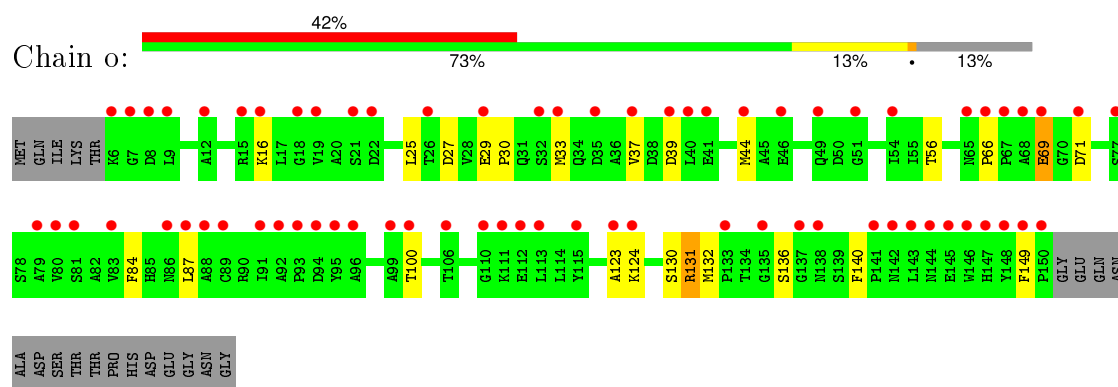
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4





F149		S77	MET
P150	GLY	S78	GLN
	GLU	A79	ILE
	GLN	V80	LVS
	ASN	S81	THR
	ALA	A82	K6
	ASP	F84	G7
	SER		D8
	THR	L87	L9
	PRO	A88	V10
	HIS	C89	R11
	ASP	N90	A12
	GLU	I91	
	ASN	A92	K15
	GLY	P93	R16
	ASN	E98	S21
GLY		A99	D22
		K102	L25
		T105	T26
		A107	D27
		K108	V28
		Y109	E29
		L113	P30
		L114	Q31
		Y115	S32
		K116	M33
		Q117	Q34
		T118	D35
		A119	A36
		R122	V37
		A123	D38
		K124	D39
		R125	L40
		A126	M44
		P127	G53
		Y128	I54
		P129	I55
		S130	T56
		R131	G57
		M132	Y58
		P133	V59
		T134	D63
		G135	E64
		S136	M65
		F140	P67
		P141	A68
		N142	E69
		L143	G70
		N144	D71
		E145	D72
		W146	H73
		H147	G74
		Y148	L75
			B76


[illegible][illegible]

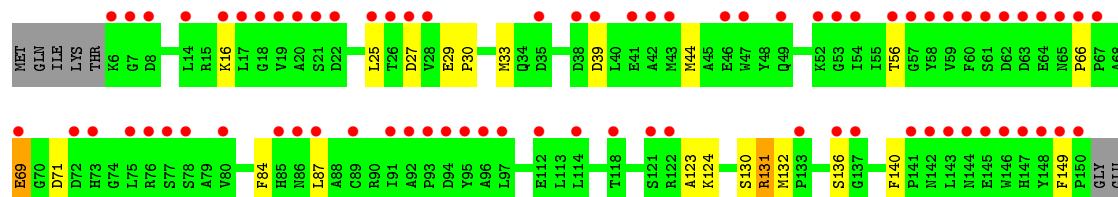
R76	R77	R80	F84	H85	H86	L87	K16	L17	G18	V19	A20	S21	D22	A23	T24	I25	T26	D27	E29	F30	G31	S32	P33	G34	D35	A36	V37	D38	D39	L40	E41	A42	P43	N44	G53	I54	L55	V56	G57	F60	S61	D62	D63	E64	N65	P66	E69	G70	D71	H72	A73	H74	G75	GLY	GLY
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GLN  
ASN  
ALA  
ASP  
SER  
THR  
THR  
PRO  
HIS  
ASP  
GLU  
GLY  
ASN  
GLY


• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

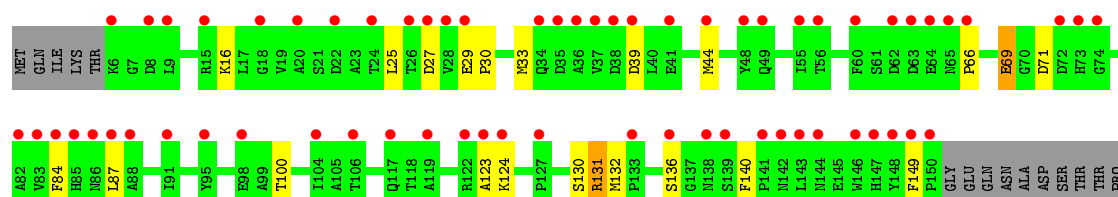
Chain t: 



GLN  
ASN  
ALA  
ASP  
SER  
THR  
THR  
PRO  
HIS  
ASP  
GLU  
GLY  
ASN  
GLY


• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

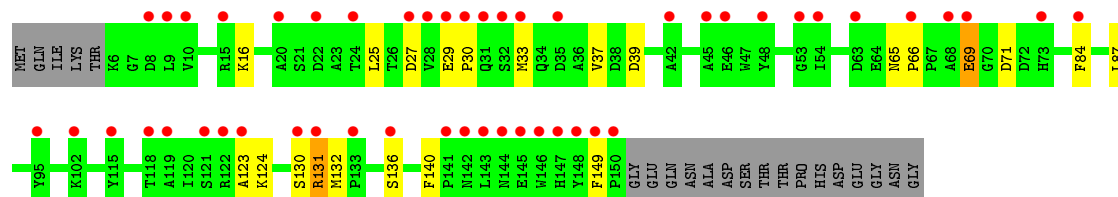
Chain u: 



HIS  
ASP  
GLU  
GLY  
ASN  
GLY

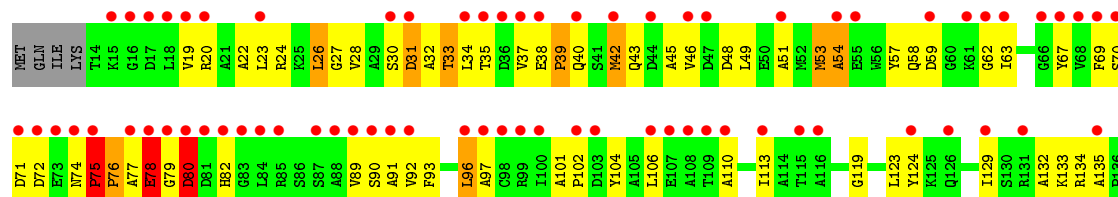
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain v: 

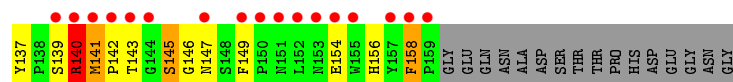


• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

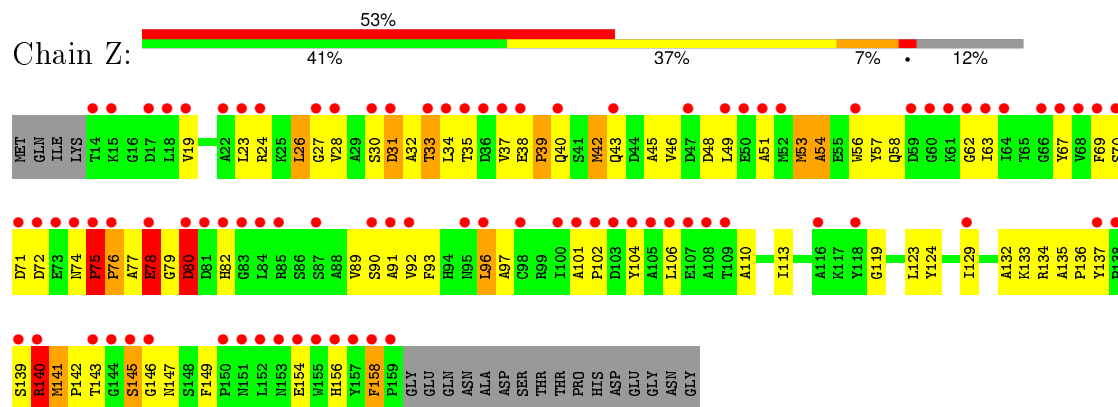
Chain Y: 



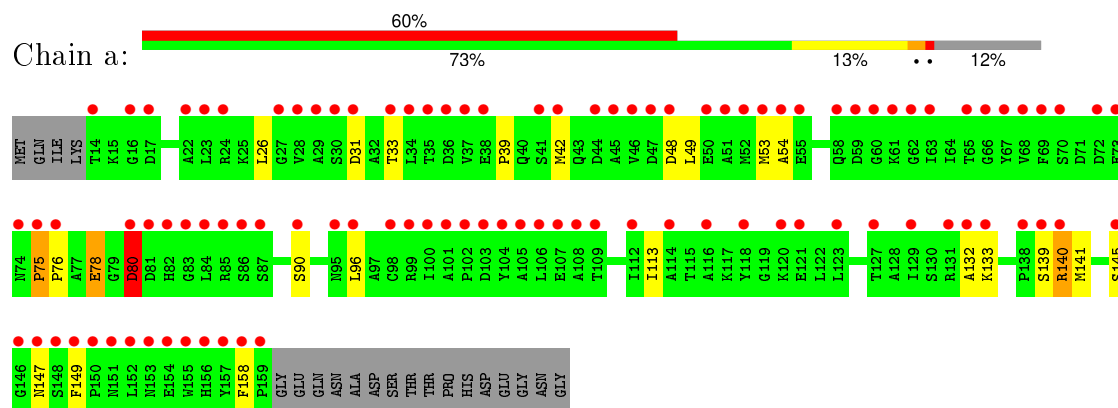




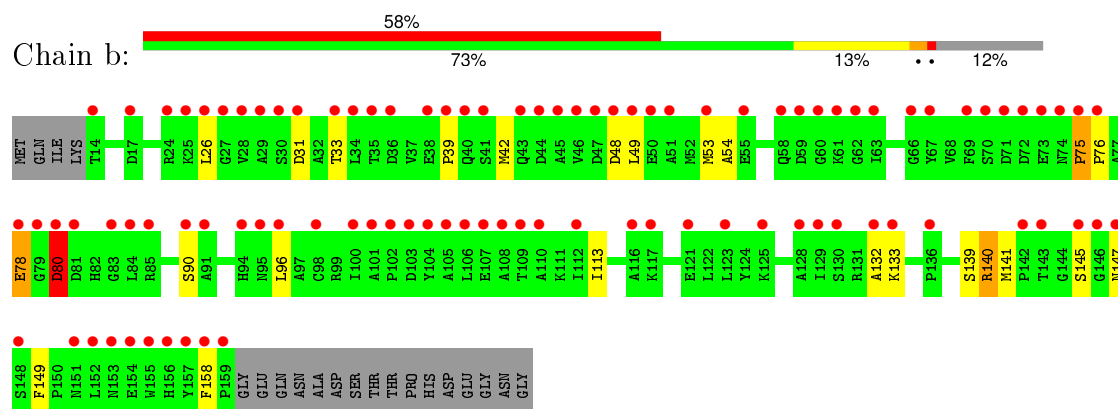
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



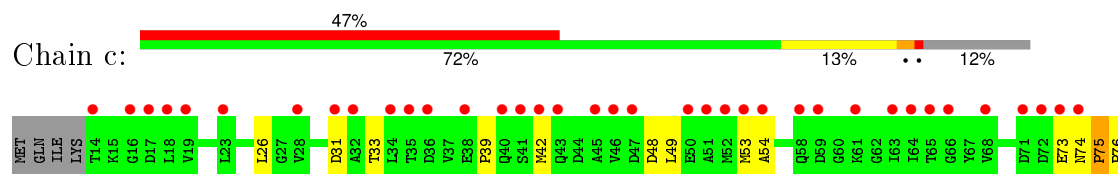
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



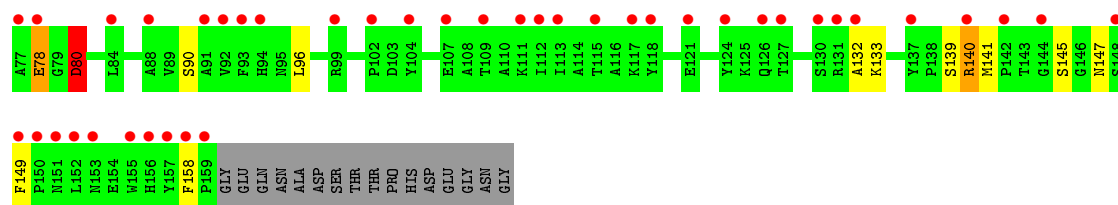
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



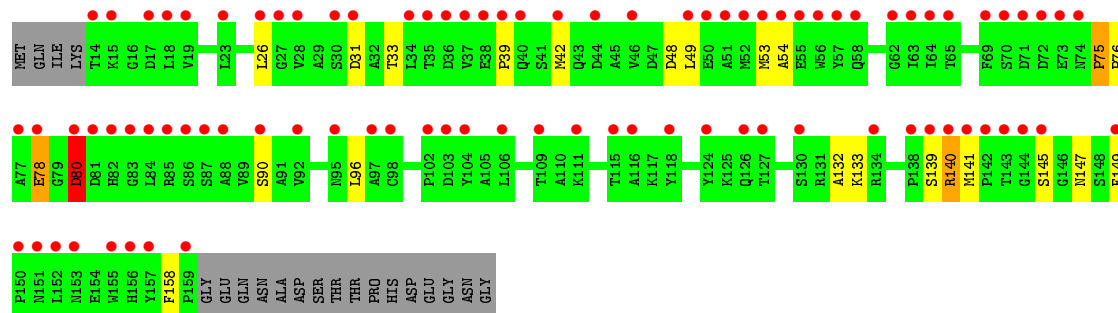
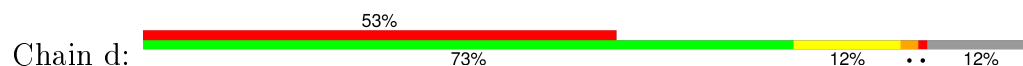
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



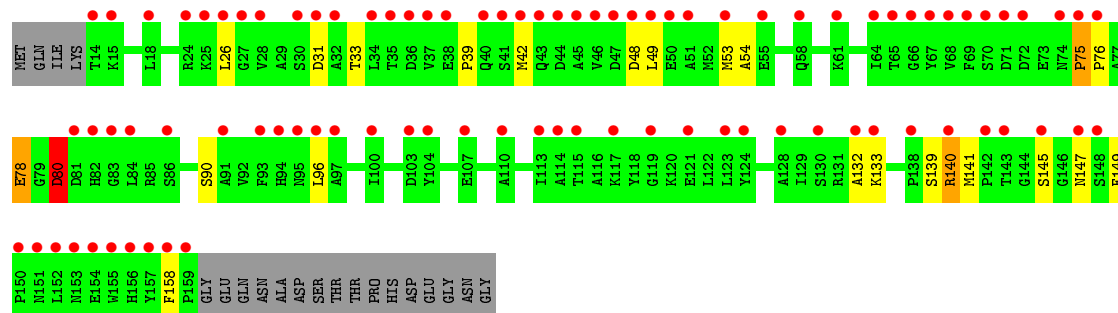
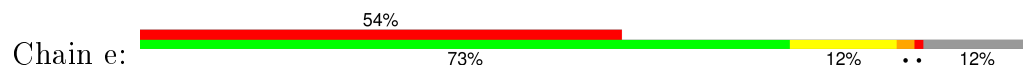




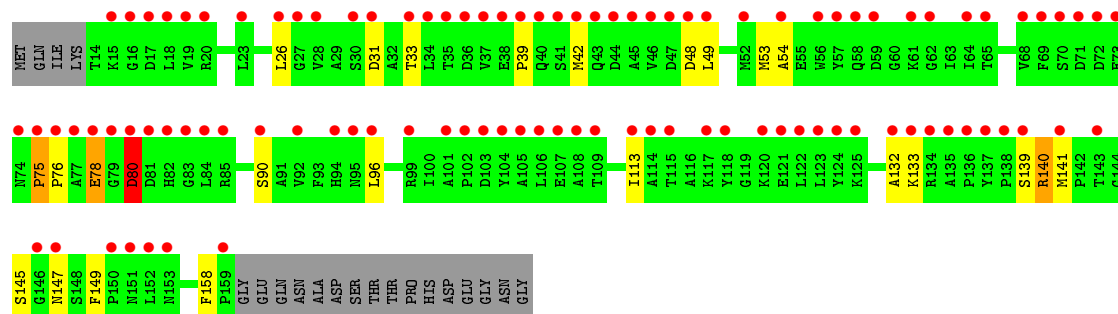
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



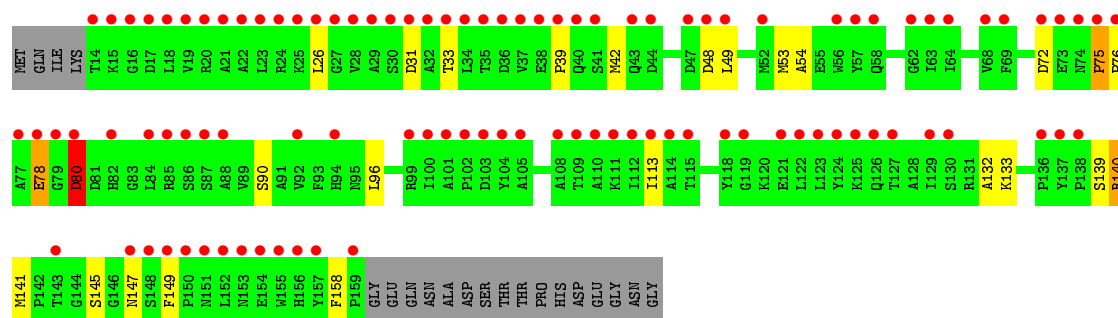
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



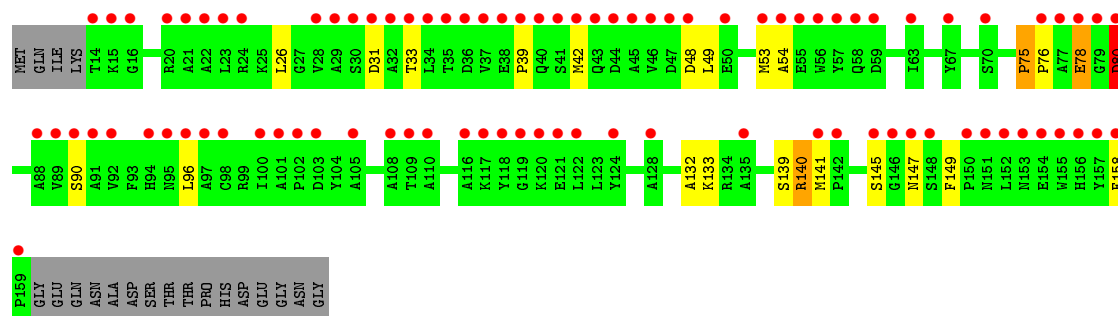
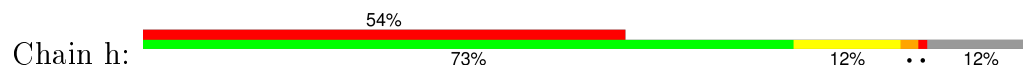
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



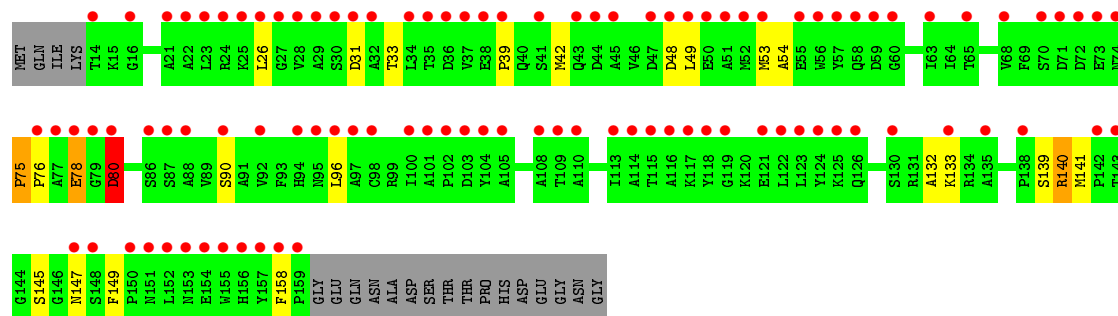
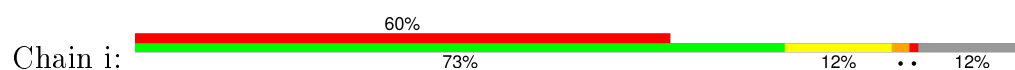




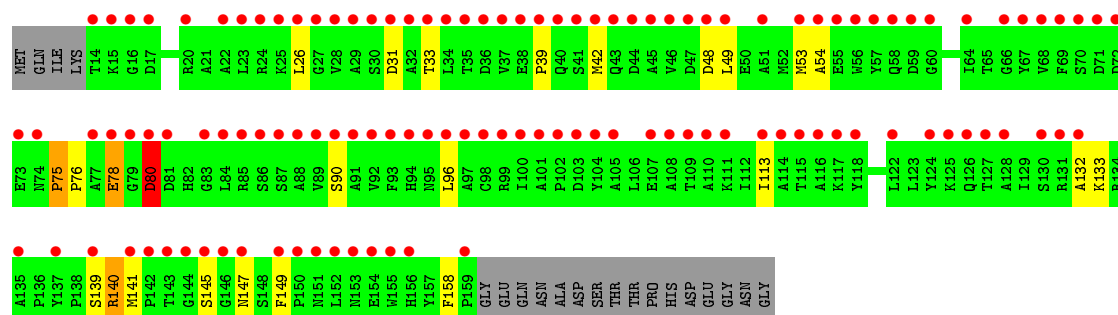
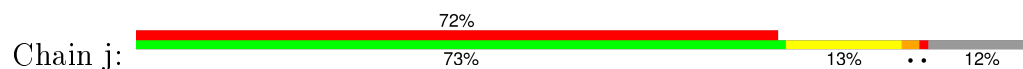
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.17Å 253.28Å 282.73Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	19.99 – 3.25 78.75 – 3.23	Depositor EDS
% Data completeness (in resolution range)	59.7 (19.99-3.25) 91.6 (78.75-3.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.222 , 0.236 0.282 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	1.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 107.8	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	36 of 349411 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	135120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.35	0/4635	0.54	0/6265
1	B	0.35	0/4635	0.54	0/6265
1	C	0.35	0/4635	0.54	0/6265
1	D	0.35	0/4635	0.54	0/6265
1	E	0.35	0/4635	0.54	0/6265
1	F	0.35	0/4635	0.54	0/6265
1	G	0.35	0/4635	0.54	0/6265
1	H	0.35	0/4635	0.54	0/6265
1	I	0.35	0/4635	0.54	0/6265
1	J	0.35	0/4635	0.54	0/6265
1	K	0.35	0/4635	0.54	0/6265
1	L	0.35	0/4635	0.54	0/6265
1	M	0.31	0/4646	0.51	0/6278
1	N	0.32	0/4646	0.51	0/6278
1	O	0.32	0/4646	0.50	0/6278
1	P	0.32	0/4646	0.51	0/6278
1	Q	0.32	0/4646	0.51	0/6278
1	R	0.32	0/4646	0.51	0/6278
1	S	0.31	0/4646	0.51	0/6278
1	T	0.31	0/4646	0.50	0/6278
1	U	0.31	0/4646	0.51	0/6278
1	V	0.32	0/4646	0.51	0/6278
1	W	0.31	0/4646	0.55	2/6278 (0.0%)
1	X	0.31	0/4646	0.50	0/6278
2	Y	0.37	0/1067	0.84	4/1452 (0.3%)
2	Z	0.37	0/1067	0.85	4/1452 (0.3%)
2	a	0.37	0/1067	0.84	4/1452 (0.3%)
2	b	0.37	0/1067	0.84	4/1452 (0.3%)
2	c	0.37	0/1067	0.84	4/1452 (0.3%)
2	d	0.37	0/1067	0.84	4/1452 (0.3%)
2	e	0.37	0/1067	0.84	4/1452 (0.3%)
2	f	0.37	0/1067	0.84	4/1452 (0.3%)
2	g	0.37	0/1067	0.84	4/1452 (0.3%)
2	h	0.37	0/1067	0.84	4/1452 (0.3%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	i	0.37	0/1067	0.85	4/1452 (0.3%)
2	j	0.37	0/1067	0.84	4/1452 (0.3%)
2	k	0.32	0/1071	0.52	0/1455
2	l	0.33	0/1071	0.52	0/1455
2	m	0.33	0/1071	0.51	0/1455
2	n	0.33	0/1071	0.51	0/1455
2	o	0.33	0/1071	0.51	0/1455
2	p	0.33	0/1071	0.51	0/1455
2	q	0.32	0/1071	0.51	0/1455
2	r	0.36	0/1071	0.51	0/1455
2	s	0.32	0/1071	0.52	0/1455
2	t	0.32	0/1071	0.51	0/1455
2	u	0.31	0/1071	0.51	0/1455
2	v	0.32	0/1071	0.51	0/1455
All	All	0.34	0/137028	0.56	50/185400 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1
1	V	0	1
1	W	0	1
1	X	0	1
All	All	0	24

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	80	ASP	N-CA-CB	17.19	141.54	110.60
2	d	80	ASP	N-CA-CB	17.18	141.52	110.60
2	Z	80	ASP	N-CA-CB	17.17	141.51	110.60
2	Y	80	ASP	N-CA-CB	17.17	141.50	110.60
2	e	80	ASP	N-CA-CB	17.17	141.50	110.60

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	231	THR	Peptide
1	N	231	THR	Peptide
1	O	231	THR	Peptide
1	P	231	THR	Peptide
1	Q	231	THR	Peptide

## 5.2 Too-close contacts [i](#)

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	A	4553	0	4351	430	0
1	B	4553	0	4351	437	2
1	C	4553	0	4351	432	4
1	D	4553	0	4351	423	0
1	E	4553	0	4351	430	0
1	F	4553	0	4351	428	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4553	0	4351	430	0
1	H	4553	0	4351	424	0
1	I	4553	0	4351	433	0
1	J	4553	0	4351	430	0
1	K	4553	0	4351	431	0
1	L	4553	0	4351	441	0
1	M	4564	0	4368	365	0
1	N	4564	0	4368	375	5
1	O	4564	0	4368	363	0
1	P	4564	0	4368	371	0
1	Q	4564	0	4368	373	0
1	R	4564	0	4368	385	0
1	S	4564	0	4368	364	3
1	T	4564	0	4368	366	0
1	U	4564	0	4368	374	0
1	V	4564	0	4368	368	0
1	W	4564	0	4368	364	1
1	X	4564	0	4368	364	0
2	Y	1048	0	957	111	0
2	Z	1048	0	957	108	0
2	a	1048	0	957	0	0
2	b	1048	0	957	0	0
2	c	1048	0	957	0	4
2	d	1048	0	957	0	0
2	e	1048	0	957	0	0
2	f	1048	0	957	0	0
2	g	1048	0	957	0	1
2	h	1048	0	957	0	0
2	i	1048	0	957	0	0
2	j	1048	0	957	0	0
2	k	1052	0	975	0	0
2	l	1052	0	975	0	0
2	m	1052	0	975	0	0
2	n	1052	0	975	0	0
2	o	1052	0	975	0	0
2	p	1052	0	975	0	0
2	q	1052	0	975	0	0
2	r	1052	0	975	0	3
2	s	1052	0	975	0	0
2	t	1052	0	975	0	0
2	u	1052	0	975	0	0
2	v	1052	0	975	0	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	0	1	0
3	B	22	0	0	1	0
3	C	22	0	0	1	0
3	D	22	0	0	1	0
3	E	22	0	0	2	0
3	F	22	0	0	2	0
3	G	22	0	0	1	0
3	H	22	0	0	2	0
3	I	22	0	0	1	0
3	J	22	0	0	2	0
3	K	22	0	0	2	0
3	L	22	0	0	2	0
3	M	21	0	0	4	0
3	N	21	0	0	4	0
3	O	21	0	0	3	0
3	P	21	0	0	5	0
3	Q	21	0	0	5	0
3	R	21	0	0	4	0
3	S	21	0	0	4	0
3	T	21	0	0	5	0
3	U	21	0	0	3	0
3	V	21	0	0	4	0
3	W	21	0	0	4	0
3	X	21	0	0	4	0
All	All	135120	0	127812	9241	13

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 42.

The worst 5 of 9241 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:Z:32:ALA:O	2:Z:33:THR:CG2	1.82	1.27
2:Z:32:ALA:O	2:Z:33:THR:HG23	1.12	1.26
2:Y:32:ALA:O	2:Y:33:THR:CG2	1.82	1.26
2:Y:32:ALA:O	2:Y:33:THR:HG23	1.12	1.24
2:Z:28:VAL:HG21	2:Z:96:LEU:CD1	1.68	1.23

The worst 5 of 13 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)
1:C:230:GLU:OE2	2:c:74:ASN:ND2[2_546]	1.06	1.14
1:N:230:GLU:N	2:r:64:GLU:OE2[2_455]	1.79	0.41
1:N:260:ASP:OD2	1:B:601:GLN:NE2[2_555]	1.79	0.41
1:C:250:ASP:OD2	2:c:74:ASN:OD1[2_546]	1.83	0.37
1:N:228:LYS:CG	2:r:64:GLU:OE1[2_455]	1.89	0.31

## 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	A	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	B	565/602 (94%)	434 (77%)	87 (15%)	44 (8%)	1	8
1	C	565/602 (94%)	434 (77%)	87 (15%)	44 (8%)	1	8
1	D	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	E	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	F	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	G	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	H	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	I	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	J	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	K	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1	9
1	L	565/602 (94%)	434 (77%)	87 (15%)	44 (8%)	1	8
1	M	565/602 (94%)	446 (79%)	81 (14%)	38 (7%)	1	12
1	N	565/602 (94%)	447 (79%)	79 (14%)	39 (7%)	1	11
1	O	565/602 (94%)	447 (79%)	80 (14%)	38 (7%)	1	12
1	P	565/602 (94%)	448 (79%)	79 (14%)	38 (7%)	1	12
1	Q	565/602 (94%)	447 (79%)	79 (14%)	39 (7%)	1	11
1	R	565/602 (94%)	448 (79%)	79 (14%)	38 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	565/602 (94%)	443 (78%)	83 (15%)	39 (7%)	1	11
1	T	565/602 (94%)	446 (79%)	81 (14%)	38 (7%)	1	12
1	U	565/602 (94%)	447 (79%)	79 (14%)	39 (7%)	1	11
1	V	565/602 (94%)	445 (79%)	82 (14%)	38 (7%)	1	12
1	W	565/602 (94%)	448 (79%)	78 (14%)	39 (7%)	1	11
1	X	565/602 (94%)	448 (79%)	78 (14%)	39 (7%)	1	11
2	Y	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	Z	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	a	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	b	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	c	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	d	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	e	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	f	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	g	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	h	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	i	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	j	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	6
2	k	143/166 (86%)	115 (80%)	17 (12%)	11 (8%)	1	9
2	l	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	9
2	m	143/166 (86%)	115 (80%)	18 (13%)	10 (7%)	1	10
2	n	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	9
2	o	143/166 (86%)	115 (80%)	17 (12%)	11 (8%)	1	9
2	p	143/166 (86%)	115 (80%)	17 (12%)	11 (8%)	1	9
2	q	143/166 (86%)	113 (79%)	19 (13%)	11 (8%)	1	9
2	r	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	9
2	s	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	9
2	t	143/166 (86%)	113 (79%)	19 (13%)	11 (8%)	1	9
2	u	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	9
2	v	143/166 (86%)	114 (80%)	19 (13%)	10 (7%)	1	10
All	All	17004/18432 (92%)	13318 (78%)	2419 (14%)	1267 (8%)	1	9



5 of 1267 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	82	PRO
1	M	263	PHE
1	M	294	ALA
1	M	462	GLU
1	M	514	TYR

### 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	A	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	B	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	C	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	D	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	E	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	F	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	G	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	H	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	I	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	J	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	K	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	L	483/510 (95%)	412 (85%)	71 (15%)	4	18
1	M	485/510 (95%)	412 (85%)	73 (15%)	3	17
1	N	485/510 (95%)	412 (85%)	73 (15%)	3	17
1	O	485/510 (95%)	413 (85%)	72 (15%)	4	18
1	P	485/510 (95%)	413 (85%)	72 (15%)	4	18
1	Q	485/510 (95%)	412 (85%)	73 (15%)	3	17
1	R	485/510 (95%)	411 (85%)	74 (15%)	3	17
1	S	485/510 (95%)	411 (85%)	74 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	485/510 (95%)	412 (85%)	73 (15%)	3	17
1	U	485/510 (95%)	413 (85%)	72 (15%)	4	18
1	V	485/510 (95%)	413 (85%)	72 (15%)	4	18
1	W	485/510 (95%)	413 (85%)	72 (15%)	4	18
1	X	485/510 (95%)	411 (85%)	74 (15%)	3	17
2	Y	98/132 (74%)	85 (87%)	13 (13%)	5	23
2	Z	98/132 (74%)	85 (87%)	13 (13%)	5	23
2	a	98/132 (74%)	84 (86%)	14 (14%)	4	19
2	b	98/132 (74%)	84 (86%)	14 (14%)	4	19
2	c	98/132 (74%)	85 (87%)	13 (13%)	5	23
2	d	98/132 (74%)	85 (87%)	13 (13%)	5	23
2	e	98/132 (74%)	85 (87%)	13 (13%)	5	23
2	f	98/132 (74%)	84 (86%)	14 (14%)	4	19
2	g	98/132 (74%)	84 (86%)	14 (14%)	4	19
2	h	98/132 (74%)	85 (87%)	13 (13%)	5	23
2	i	98/132 (74%)	85 (87%)	13 (13%)	5	23
2	j	98/132 (74%)	84 (86%)	14 (14%)	4	19
2	k	100/132 (76%)	88 (88%)	12 (12%)	6	28
2	l	100/132 (76%)	87 (87%)	13 (13%)	5	24
2	m	100/132 (76%)	88 (88%)	12 (12%)	6	28
2	n	100/132 (76%)	87 (87%)	13 (13%)	5	24
2	o	100/132 (76%)	85 (85%)	15 (15%)	3	17
2	p	100/132 (76%)	86 (86%)	14 (14%)	4	20
2	q	100/132 (76%)	88 (88%)	12 (12%)	6	28
2	r	100/132 (76%)	88 (88%)	12 (12%)	6	28
2	s	100/132 (76%)	87 (87%)	13 (13%)	5	24
2	t	100/132 (76%)	87 (87%)	13 (13%)	5	24
2	u	100/132 (76%)	87 (87%)	13 (13%)	5	24
2	v	100/132 (76%)	87 (87%)	13 (13%)	5	24
All	All	13992/15408 (91%)	11950 (85%)	2042 (15%)	4	19

5 of 2042 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	n	136	SER
1	B	301	VAL
2	Y	80	ASP
2	p	130	SER
1	A	43	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 319 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	161	ASN
1	F	530	GLN
1	L	214	GLN
1	E	214	GLN
1	F	112	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

### 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	A	552/602 (91%)	2.81	288 (52%)	0	0	22, 84, 246, 379	0
1	B	552/602 (91%)	2.87	311 (56%)	0	0	23, 85, 246, 379	0
1	C	552/602 (91%)	2.84	303 (54%)	0	0	26, 84, 246, 379	0
1	D	552/602 (91%)	2.59	266 (48%)	0	0	25, 84, 246, 379	0
1	E	552/602 (91%)	2.79	285 (51%)	0	0	25, 84, 246, 379	0
1	F	552/602 (91%)	2.72	265 (48%)	0	0	25, 84, 246, 379	0
1	G	552/602 (91%)	2.75	278 (50%)	0	0	30, 84, 246, 379	0
1	H	552/602 (91%)	2.89	288 (52%)	0	0	26, 86, 246, 379	0
1	I	552/602 (91%)	2.90	300 (54%)	0	0	31, 88, 246, 379	0
1	J	552/602 (91%)	3.00	329 (59%)	0	0	33, 96, 246, 379	0
1	K	552/602 (91%)	3.05	304 (55%)	0	0	26, 88, 245, 379	0
1	L	552/602 (91%)	3.05	312 (56%)	0	0	24, 87, 246, 379	0
1	M	552/602 (91%)	2.33	236 (42%)	0	0	15, 70, 209, 327	0
1	N	552/602 (91%)	2.19	215 (38%)	0	1	18, 69, 209, 327	0
1	O	552/602 (91%)	2.16	224 (40%)	0	1	15, 69, 209, 326	0
1	P	552/602 (91%)	2.22	236 (42%)	0	0	15, 70, 209, 327	0
1	Q	552/602 (91%)	2.25	226 (40%)	0	1	15, 69, 209, 326	0
1	R	552/602 (91%)	2.29	219 (39%)	0	1	17, 69, 209, 327	0
1	S	552/602 (91%)	2.39	248 (44%)	0	0	19, 70, 209, 326	0
1	T	552/602 (91%)	2.46	241 (43%)	0	0	15, 70, 208, 326	0
1	U	552/602 (91%)	2.61	278 (50%)	0	0	17, 69, 209, 327	0
1	V	552/602 (91%)	2.49	230 (41%)	0	0	18, 70, 209, 327	0
1	W	552/602 (91%)	2.32	249 (45%)	0	0	17, 70, 209, 326	0
1	X	552/602 (91%)	2.50	242 (43%)	0	0	14, 69, 209, 326	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
2	Y	146/166 (87%)	3.81	88 (60%)	0	0	38, 75, 221, 304	0
2	Z	146/166 (87%)	3.67	88 (60%)	0	0	37, 73, 222, 304	0
2	a	146/166 (87%)	3.64	100 (68%)	0	0	37, 77, 221, 304	0
2	b	146/166 (87%)	3.64	96 (65%)	0	0	39, 72, 221, 304	0
2	c	146/166 (87%)	2.66	78 (53%)	0	0	39, 72, 222, 305	0
2	d	146/166 (87%)	3.07	88 (60%)	0	0	35, 72, 222, 304	0
2	e	146/166 (87%)	3.12	89 (60%)	0	0	37, 73, 220, 304	0
2	f	146/166 (87%)	3.68	100 (68%)	0	0	39, 74, 222, 304	0
2	g	146/166 (87%)	3.69	101 (69%)	0	0	44, 75, 221, 304	0
2	h	146/166 (87%)	3.67	89 (60%)	0	0	38, 75, 221, 305	0
2	i	146/166 (87%)	3.52	100 (68%)	0	0	40, 75, 221, 304	0
2	j	146/166 (87%)	4.19	119 (81%)	0	0	36, 75, 222, 305	0
2	k	145/166 (87%)	2.88	72 (49%)	0	0	25, 57, 204, 314	0
2	l	145/166 (87%)	2.82	77 (53%)	0	0	28, 56, 204, 314	0
2	m	145/166 (87%)	3.28	79 (54%)	0	0	30, 59, 203, 314	0
2	n	145/166 (87%)	2.75	65 (44%)	0	0	23, 55, 204, 314	0
2	o	145/166 (87%)	2.58	70 (48%)	0	0	26, 57, 204, 314	0
2	p	145/166 (87%)	2.96	75 (51%)	0	0	27, 57, 204, 314	0
2	q	145/166 (87%)	2.75	68 (46%)	0	0	29, 58, 204, 314	0
2	r	145/166 (87%)	2.65	65 (44%)	0	0	26, 57, 205, 314	0
2	s	145/166 (87%)	2.80	77 (53%)	0	0	30, 58, 204, 314	0
2	t	145/166 (87%)	2.90	76 (52%)	0	0	31, 58, 204, 314	0
2	u	145/166 (87%)	2.54	64 (44%)	0	0	30, 58, 204, 314	0
2	v	145/166 (87%)	1.99	49 (33%)	0	1	29, 57, 204, 314	0
All	All	16740/18432 (90%)	2.71	8346 (49%)	0	0	14, 76, 228, 379	0

The worst 5 of 8346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	151	ASN	38.0
2	Y	152	LEU	36.1
1	D	240	THR	33.9
1	K	210	PRO	31.5
2	Y	150	PRO	30.5



## 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.