



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:42 PM BST

PDB ID : 6IGC  
Title : Crystal structure of HPV58/33/52 chimeric L1 pentamer  
Authors : Li, Z.H.; Song, S.; He, M.Z.; Gu, Y.; Li, S.W.  
Deposited on : 2018-09-25  
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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	:	2.13
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)	:	2.13

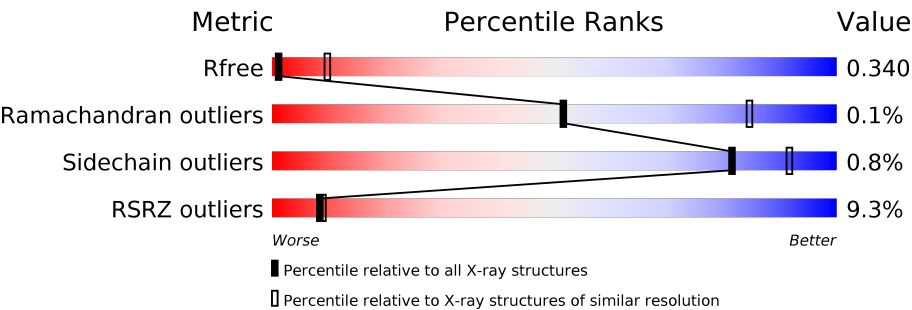
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	A	524	
1	B	524	
1	C	524	
1	D	524	
1	E	524	
1	F	524	
1	G	524	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain		
1	H	524	15%	79%	21%
1	I	524	17%	79%	20%
1	J	524	5%	79%	20%
1	K	524	%	78%	21%
1	L	524		79%	21%
1	M	524		78%	21%
1	N	524		78%	21%
1	O	524		79%	20%
1	P	524		78%	21%
1	Q	524		79%	21%
1	R	524		79%	21%
1	S	524	%	79%	20%
1	T	524		79%	20%
1	U	524	9%	78%	21%
1	V	524	15%	79%	21%
1	W	524	6%	78%	21%
1	X	524	23%	78%	20%
1	Y	524	20%	79%	20%
1	Z	524	8%	78%	21%
1	a	524	11%	79%	21%
1	b	524	6%	79%	21%
1	c	524	10%	79%	20%
1	d	524	18%	79%	20%
1	e	524	30%	78%	21%
1	f	524	5%	79%	21%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	g	524	<div><div></div><div>34%78%21%</div></div>
1	h	524	<div><div></div><div>33%79%20%</div></div>
1	i	524	<div><div></div><div>8%79%20%</div></div>
1	j	524	<div><div></div><div>%78%21%</div></div>
1	k	524	<div><div></div><div>78%21%</div></div>
1	l	524	<div><div></div><div>79%21%</div></div>
1	m	524	<div><div></div><div>%79%20%</div></div>
1	n	524	<div><div></div><div>2%79%20%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 133128 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	1	0
			3352	2137	557	638	20			
1	B	413	Total	C	N	O	S	0	1	0
			3307	2113	547	627	20			
1	C	416	Total	C	N	O	S	0	0	0
			3327	2124	552	632	19			
1	D	416	Total	C	N	O	S	0	1	0
			3329	2125	553	631	20			
1	E	414	Total	C	N	O	S	0	1	0
			3307	2110	549	628	20			
1	F	416	Total	C	N	O	S	0	1	0
			3327	2125	551	631	20			
1	G	414	Total	C	N	O	S	0	1	0
			3316	2119	549	628	20			
1	H	415	Total	C	N	O	S	0	1	0
			3322	2122	550	630	20			
1	I	418	Total	C	N	O	S	0	1	0
			3336	2130	554	632	20			
1	J	420	Total	C	N	O	S	0	1	0
			3352	2138	558	636	20			
1	K	415	Total	C	N	O	S	0	1	0
			3318	2119	549	630	20			
1	L	414	Total	C	N	O	S	0	1	0
			3316	2119	549	628	20			
1	M	415	Total	C	N	O	S	0	1	0
			3322	2122	550	630	20			
1	N	416	Total	C	N	O	S	0	1	0
			3323	2123	551	629	20			
1	O	420	Total	C	N	O	S	0	1	0
			3352	2138	558	636	20			
1	P	415	Total	C	N	O	S	0	1	0
			3318	2119	549	630	20			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	414	Total	C	N	O	S	0	1	0
			3316	2119	549	628	20			
1	R	415	Total	C	N	O	S	0	1	0
			3322	2122	550	630	20			
1	S	418	Total	C	N	O	S	0	1	0
			3336	2130	554	632	20			
1	T	420	Total	C	N	O	S	0	1	0
			3352	2138	558	636	20			
1	U	414	Total	C	N	O	S	0	1	0
			3311	2114	548	629	20			
1	V	414	Total	C	N	O	S	0	1	0
			3316	2119	549	628	20			
1	W	415	Total	C	N	O	S	0	1	0
			3322	2122	550	630	20			
1	X	418	Total	C	N	O	S	0	1	0
			3336	2130	554	632	20			
1	Y	420	Total	C	N	O	S	0	1	0
			3352	2138	558	636	20			
1	Z	415	Total	C	N	O	S	0	1	0
			3318	2119	549	630	20			
1	a	414	Total	C	N	O	S	0	1	0
			3316	2119	549	628	20			
1	b	415	Total	C	N	O	S	0	1	0
			3322	2122	550	630	20			
1	c	418	Total	C	N	O	S	0	1	0
			3336	2130	554	632	20			
1	d	420	Total	C	N	O	S	0	1	0
			3352	2138	558	636	20			
1	e	416	Total	C	N	O	S	0	1	0
			3327	2125	551	631	20			
1	f	414	Total	C	N	O	S	0	1	0
			3316	2119	549	628	20			
1	g	415	Total	C	N	O	S	0	1	0
			3322	2122	550	630	20			
1	h	418	Total	C	N	O	S	0	1	0
			3336	2130	554	632	20			
1	i	420	Total	C	N	O	S	0	1	0
			3352	2138	558	636	20			
1	j	415	Total	C	N	O	S	0	1	0
			3318	2119	549	630	20			
1	k	414	Total	C	N	O	S	0	1	0
			3316	2119	549	628	20			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	415	Total	C	N	O	S	0	1	0
			3322	2122	550	630	20			
1	m	418	Total	C	N	O	S	0	1	0
			3336	2130	554	632	20			
1	n	420	Total	C	N	O	S	0	1	0
			3352	2138	558	636	20			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P26535
A	56	THR	ASN	engineered mutation	UNP P26535
A	58	ALA	ASN	engineered mutation	UNP P26535
A	61	LEU	VAL	engineered mutation	UNP P26535
A	176	SER	CYS	engineered mutation	UNP P26535
A	349	LYS	THR	engineered mutation	UNP P26535
A	352	SER	GLY	engineered mutation	UNP P26535
A	357	GLU	ASP	engineered mutation	UNP P26535
B	54	ASN	SER	engineered mutation	UNP P26535
B	56	THR	ASN	engineered mutation	UNP P26535
B	58	ALA	ASN	engineered mutation	UNP P26535
B	61	LEU	VAL	engineered mutation	UNP P26535
B	176	SER	CYS	engineered mutation	UNP P26535
B	349	LYS	THR	engineered mutation	UNP P26535
B	352	SER	GLY	engineered mutation	UNP P26535
B	357	GLU	ASP	engineered mutation	UNP P26535
C	54	ASN	SER	engineered mutation	UNP P26535
C	56	THR	ASN	engineered mutation	UNP P26535
C	58	ALA	ASN	engineered mutation	UNP P26535
C	61	LEU	VAL	engineered mutation	UNP P26535
C	176	SER	CYS	engineered mutation	UNP P26535
C	349	LYS	THR	engineered mutation	UNP P26535
C	352	SER	GLY	engineered mutation	UNP P26535
C	357	GLU	ASP	engineered mutation	UNP P26535
D	54	ASN	SER	engineered mutation	UNP P26535
D	56	THR	ASN	engineered mutation	UNP P26535
D	58	ALA	ASN	engineered mutation	UNP P26535
D	61	LEU	VAL	engineered mutation	UNP P26535
D	176	SER	CYS	engineered mutation	UNP P26535
D	349	LYS	THR	engineered mutation	UNP P26535
D	352	SER	GLY	engineered mutation	UNP P26535
D	357	GLU	ASP	engineered mutation	UNP P26535

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	54	ASN	SER	engineered mutation	UNP P26535
E	56	THR	ASN	engineered mutation	UNP P26535
E	58	ALA	ASN	engineered mutation	UNP P26535
E	61	LEU	VAL	engineered mutation	UNP P26535
E	176	SER	CYS	engineered mutation	UNP P26535
E	349	LYS	THR	engineered mutation	UNP P26535
E	352	SER	GLY	engineered mutation	UNP P26535
E	357	GLU	ASP	engineered mutation	UNP P26535
F	54	ASN	SER	engineered mutation	UNP P26535
F	56	THR	ASN	engineered mutation	UNP P26535
F	58	ALA	ASN	engineered mutation	UNP P26535
F	61	LEU	VAL	engineered mutation	UNP P26535
F	176	SER	CYS	engineered mutation	UNP P26535
F	349	LYS	THR	engineered mutation	UNP P26535
F	352	SER	GLY	engineered mutation	UNP P26535
F	357	GLU	ASP	engineered mutation	UNP P26535
G	54	ASN	SER	engineered mutation	UNP P26535
G	56	THR	ASN	engineered mutation	UNP P26535
G	58	ALA	ASN	engineered mutation	UNP P26535
G	61	LEU	VAL	engineered mutation	UNP P26535
G	176	SER	CYS	engineered mutation	UNP P26535
G	349	LYS	THR	engineered mutation	UNP P26535
G	352	SER	GLY	engineered mutation	UNP P26535
G	357	GLU	ASP	engineered mutation	UNP P26535
H	54	ASN	SER	engineered mutation	UNP P26535
H	56	THR	ASN	engineered mutation	UNP P26535
H	58	ALA	ASN	engineered mutation	UNP P26535
H	61	LEU	VAL	engineered mutation	UNP P26535
H	176	SER	CYS	engineered mutation	UNP P26535
H	349	LYS	THR	engineered mutation	UNP P26535
H	352	SER	GLY	engineered mutation	UNP P26535
H	357	GLU	ASP	engineered mutation	UNP P26535
I	54	ASN	SER	engineered mutation	UNP P26535
I	56	THR	ASN	engineered mutation	UNP P26535
I	58	ALA	ASN	engineered mutation	UNP P26535
I	61	LEU	VAL	engineered mutation	UNP P26535
I	176	SER	CYS	engineered mutation	UNP P26535
I	349	LYS	THR	engineered mutation	UNP P26535
I	352	SER	GLY	engineered mutation	UNP P26535
I	357	GLU	ASP	engineered mutation	UNP P26535
J	54	ASN	SER	engineered mutation	UNP P26535
J	56	THR	ASN	engineered mutation	UNP P26535

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	58	ALA	ASN	engineered mutation	UNP P26535
J	61	LEU	VAL	engineered mutation	UNP P26535
J	176	SER	CYS	engineered mutation	UNP P26535
J	349	LYS	THR	engineered mutation	UNP P26535
J	352	SER	GLY	engineered mutation	UNP P26535
J	357	GLU	ASP	engineered mutation	UNP P26535
K	54	ASN	SER	engineered mutation	UNP P26535
K	56	THR	ASN	engineered mutation	UNP P26535
K	58	ALA	ASN	engineered mutation	UNP P26535
K	61	LEU	VAL	engineered mutation	UNP P26535
K	176	SER	CYS	engineered mutation	UNP P26535
K	349	LYS	THR	engineered mutation	UNP P26535
K	352	SER	GLY	engineered mutation	UNP P26535
K	357	GLU	ASP	engineered mutation	UNP P26535
L	54	ASN	SER	engineered mutation	UNP P26535
L	56	THR	ASN	engineered mutation	UNP P26535
L	58	ALA	ASN	engineered mutation	UNP P26535
L	61	LEU	VAL	engineered mutation	UNP P26535
L	176	SER	CYS	engineered mutation	UNP P26535
L	349	LYS	THR	engineered mutation	UNP P26535
L	352	SER	GLY	engineered mutation	UNP P26535
L	357	GLU	ASP	engineered mutation	UNP P26535
M	54	ASN	SER	engineered mutation	UNP P26535
M	56	THR	ASN	engineered mutation	UNP P26535
M	58	ALA	ASN	engineered mutation	UNP P26535
M	61	LEU	VAL	engineered mutation	UNP P26535
M	176	SER	CYS	engineered mutation	UNP P26535
M	349	LYS	THR	engineered mutation	UNP P26535
M	352	SER	GLY	engineered mutation	UNP P26535
M	357	GLU	ASP	engineered mutation	UNP P26535
N	54	ASN	SER	engineered mutation	UNP P26535
N	56	THR	ASN	engineered mutation	UNP P26535
N	58	ALA	ASN	engineered mutation	UNP P26535
N	61	LEU	VAL	engineered mutation	UNP P26535
N	176	SER	CYS	engineered mutation	UNP P26535
N	349	LYS	THR	engineered mutation	UNP P26535
N	352	SER	GLY	engineered mutation	UNP P26535
N	357	GLU	ASP	engineered mutation	UNP P26535
O	54	ASN	SER	engineered mutation	UNP P26535
O	56	THR	ASN	engineered mutation	UNP P26535
O	58	ALA	ASN	engineered mutation	UNP P26535
O	61	LEU	VAL	engineered mutation	UNP P26535

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
O	176	SER	CYS	engineered mutation	UNP P26535
O	349	LYS	THR	engineered mutation	UNP P26535
O	352	SER	GLY	engineered mutation	UNP P26535
O	357	GLU	ASP	engineered mutation	UNP P26535
P	54	ASN	SER	engineered mutation	UNP P26535
P	56	THR	ASN	engineered mutation	UNP P26535
P	58	ALA	ASN	engineered mutation	UNP P26535
P	61	LEU	VAL	engineered mutation	UNP P26535
P	176	SER	CYS	engineered mutation	UNP P26535
P	349	LYS	THR	engineered mutation	UNP P26535
P	352	SER	GLY	engineered mutation	UNP P26535
P	357	GLU	ASP	engineered mutation	UNP P26535
Q	54	ASN	SER	engineered mutation	UNP P26535
Q	56	THR	ASN	engineered mutation	UNP P26535
Q	58	ALA	ASN	engineered mutation	UNP P26535
Q	61	LEU	VAL	engineered mutation	UNP P26535
Q	176	SER	CYS	engineered mutation	UNP P26535
Q	349	LYS	THR	engineered mutation	UNP P26535
Q	352	SER	GLY	engineered mutation	UNP P26535
Q	357	GLU	ASP	engineered mutation	UNP P26535
R	54	ASN	SER	engineered mutation	UNP P26535
R	56	THR	ASN	engineered mutation	UNP P26535
R	58	ALA	ASN	engineered mutation	UNP P26535
R	61	LEU	VAL	engineered mutation	UNP P26535
R	176	SER	CYS	engineered mutation	UNP P26535
R	349	LYS	THR	engineered mutation	UNP P26535
R	352	SER	GLY	engineered mutation	UNP P26535
R	357	GLU	ASP	engineered mutation	UNP P26535
S	54	ASN	SER	engineered mutation	UNP P26535
S	56	THR	ASN	engineered mutation	UNP P26535
S	58	ALA	ASN	engineered mutation	UNP P26535
S	61	LEU	VAL	engineered mutation	UNP P26535
S	176	SER	CYS	engineered mutation	UNP P26535
S	349	LYS	THR	engineered mutation	UNP P26535
S	352	SER	GLY	engineered mutation	UNP P26535
S	357	GLU	ASP	engineered mutation	UNP P26535
T	54	ASN	SER	engineered mutation	UNP P26535
T	56	THR	ASN	engineered mutation	UNP P26535
T	58	ALA	ASN	engineered mutation	UNP P26535
T	61	LEU	VAL	engineered mutation	UNP P26535
T	176	SER	CYS	engineered mutation	UNP P26535
T	349	LYS	THR	engineered mutation	UNP P26535

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	352	SER	GLY	engineered mutation	UNP P26535
T	357	GLU	ASP	engineered mutation	UNP P26535
U	54	ASN	SER	engineered mutation	UNP P26535
U	56	THR	ASN	engineered mutation	UNP P26535
U	58	ALA	ASN	engineered mutation	UNP P26535
U	61	LEU	VAL	engineered mutation	UNP P26535
U	176	SER	CYS	engineered mutation	UNP P26535
U	349	LYS	THR	engineered mutation	UNP P26535
U	352	SER	GLY	engineered mutation	UNP P26535
U	357	GLU	ASP	engineered mutation	UNP P26535
V	54	ASN	SER	engineered mutation	UNP P26535
V	56	THR	ASN	engineered mutation	UNP P26535
V	58	ALA	ASN	engineered mutation	UNP P26535
V	61	LEU	VAL	engineered mutation	UNP P26535
V	176	SER	CYS	engineered mutation	UNP P26535
V	349	LYS	THR	engineered mutation	UNP P26535
V	352	SER	GLY	engineered mutation	UNP P26535
V	357	GLU	ASP	engineered mutation	UNP P26535
W	54	ASN	SER	engineered mutation	UNP P26535
W	56	THR	ASN	engineered mutation	UNP P26535
W	58	ALA	ASN	engineered mutation	UNP P26535
W	61	LEU	VAL	engineered mutation	UNP P26535
W	176	SER	CYS	engineered mutation	UNP P26535
W	349	LYS	THR	engineered mutation	UNP P26535
W	352	SER	GLY	engineered mutation	UNP P26535
W	357	GLU	ASP	engineered mutation	UNP P26535
X	54	ASN	SER	engineered mutation	UNP P26535
X	56	THR	ASN	engineered mutation	UNP P26535
X	58	ALA	ASN	engineered mutation	UNP P26535
X	61	LEU	VAL	engineered mutation	UNP P26535
X	176	SER	CYS	engineered mutation	UNP P26535
X	349	LYS	THR	engineered mutation	UNP P26535
X	352	SER	GLY	engineered mutation	UNP P26535
X	357	GLU	ASP	engineered mutation	UNP P26535
Y	54	ASN	SER	engineered mutation	UNP P26535
Y	56	THR	ASN	engineered mutation	UNP P26535
Y	58	ALA	ASN	engineered mutation	UNP P26535
Y	61	LEU	VAL	engineered mutation	UNP P26535
Y	176	SER	CYS	engineered mutation	UNP P26535
Y	349	LYS	THR	engineered mutation	UNP P26535
Y	352	SER	GLY	engineered mutation	UNP P26535
Y	357	GLU	ASP	engineered mutation	UNP P26535

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
Z	54	ASN	SER	engineered mutation	UNP P26535
Z	56	THR	ASN	engineered mutation	UNP P26535
Z	58	ALA	ASN	engineered mutation	UNP P26535
Z	61	LEU	VAL	engineered mutation	UNP P26535
Z	176	SER	CYS	engineered mutation	UNP P26535
Z	349	LYS	THR	engineered mutation	UNP P26535
Z	352	SER	GLY	engineered mutation	UNP P26535
Z	357	GLU	ASP	engineered mutation	UNP P26535
a	54	ASN	SER	engineered mutation	UNP P26535
a	56	THR	ASN	engineered mutation	UNP P26535
a	58	ALA	ASN	engineered mutation	UNP P26535
a	61	LEU	VAL	engineered mutation	UNP P26535
a	176	SER	CYS	engineered mutation	UNP P26535
a	349	LYS	THR	engineered mutation	UNP P26535
a	352	SER	GLY	engineered mutation	UNP P26535
a	357	GLU	ASP	engineered mutation	UNP P26535
b	54	ASN	SER	engineered mutation	UNP P26535
b	56	THR	ASN	engineered mutation	UNP P26535
b	58	ALA	ASN	engineered mutation	UNP P26535
b	61	LEU	VAL	engineered mutation	UNP P26535
b	176	SER	CYS	engineered mutation	UNP P26535
b	349	LYS	THR	engineered mutation	UNP P26535
b	352	SER	GLY	engineered mutation	UNP P26535
b	357	GLU	ASP	engineered mutation	UNP P26535
c	54	ASN	SER	engineered mutation	UNP P26535
c	56	THR	ASN	engineered mutation	UNP P26535
c	58	ALA	ASN	engineered mutation	UNP P26535
c	61	LEU	VAL	engineered mutation	UNP P26535
c	176	SER	CYS	engineered mutation	UNP P26535
c	349	LYS	THR	engineered mutation	UNP P26535
c	352	SER	GLY	engineered mutation	UNP P26535
c	357	GLU	ASP	engineered mutation	UNP P26535
d	54	ASN	SER	engineered mutation	UNP P26535
d	56	THR	ASN	engineered mutation	UNP P26535
d	58	ALA	ASN	engineered mutation	UNP P26535
d	61	LEU	VAL	engineered mutation	UNP P26535
d	176	SER	CYS	engineered mutation	UNP P26535
d	349	LYS	THR	engineered mutation	UNP P26535
d	352	SER	GLY	engineered mutation	UNP P26535
d	357	GLU	ASP	engineered mutation	UNP P26535
e	54	ASN	SER	engineered mutation	UNP P26535
e	56	THR	ASN	engineered mutation	UNP P26535

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
e	58	ALA	ASN	engineered mutation	UNP P26535
e	61	LEU	VAL	engineered mutation	UNP P26535
e	176	SER	CYS	engineered mutation	UNP P26535
e	349	LYS	THR	engineered mutation	UNP P26535
e	352	SER	GLY	engineered mutation	UNP P26535
e	357	GLU	ASP	engineered mutation	UNP P26535
f	54	ASN	SER	engineered mutation	UNP P26535
f	56	THR	ASN	engineered mutation	UNP P26535
f	58	ALA	ASN	engineered mutation	UNP P26535
f	61	LEU	VAL	engineered mutation	UNP P26535
f	176	SER	CYS	engineered mutation	UNP P26535
f	349	LYS	THR	engineered mutation	UNP P26535
f	352	SER	GLY	engineered mutation	UNP P26535
f	357	GLU	ASP	engineered mutation	UNP P26535
g	54	ASN	SER	engineered mutation	UNP P26535
g	56	THR	ASN	engineered mutation	UNP P26535
g	58	ALA	ASN	engineered mutation	UNP P26535
g	61	LEU	VAL	engineered mutation	UNP P26535
g	176	SER	CYS	engineered mutation	UNP P26535
g	349	LYS	THR	engineered mutation	UNP P26535
g	352	SER	GLY	engineered mutation	UNP P26535
g	357	GLU	ASP	engineered mutation	UNP P26535
h	54	ASN	SER	engineered mutation	UNP P26535
h	56	THR	ASN	engineered mutation	UNP P26535
h	58	ALA	ASN	engineered mutation	UNP P26535
h	61	LEU	VAL	engineered mutation	UNP P26535
h	176	SER	CYS	engineered mutation	UNP P26535
h	349	LYS	THR	engineered mutation	UNP P26535
h	352	SER	GLY	engineered mutation	UNP P26535
h	357	GLU	ASP	engineered mutation	UNP P26535
i	54	ASN	SER	engineered mutation	UNP P26535
i	56	THR	ASN	engineered mutation	UNP P26535
i	58	ALA	ASN	engineered mutation	UNP P26535
i	61	LEU	VAL	engineered mutation	UNP P26535
i	176	SER	CYS	engineered mutation	UNP P26535
i	349	LYS	THR	engineered mutation	UNP P26535
i	352	SER	GLY	engineered mutation	UNP P26535
i	357	GLU	ASP	engineered mutation	UNP P26535
j	54	ASN	SER	engineered mutation	UNP P26535
j	56	THR	ASN	engineered mutation	UNP P26535
j	58	ALA	ASN	engineered mutation	UNP P26535
j	61	LEU	VAL	engineered mutation	UNP P26535

*Continued on next page...*

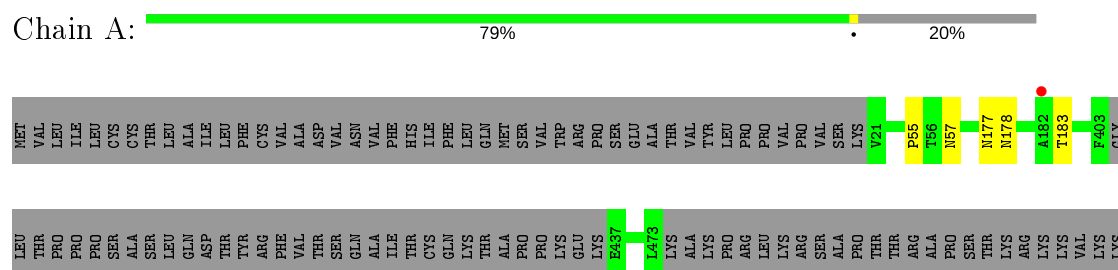
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
j	176	SER	CYS	engineered mutation	UNP P26535
j	349	LYS	THR	engineered mutation	UNP P26535
j	352	SER	GLY	engineered mutation	UNP P26535
j	357	GLU	ASP	engineered mutation	UNP P26535
k	54	ASN	SER	engineered mutation	UNP P26535
k	56	THR	ASN	engineered mutation	UNP P26535
k	58	ALA	ASN	engineered mutation	UNP P26535
k	61	LEU	VAL	engineered mutation	UNP P26535
k	176	SER	CYS	engineered mutation	UNP P26535
k	349	LYS	THR	engineered mutation	UNP P26535
k	352	SER	GLY	engineered mutation	UNP P26535
k	357	GLU	ASP	engineered mutation	UNP P26535
l	54	ASN	SER	engineered mutation	UNP P26535
l	56	THR	ASN	engineered mutation	UNP P26535
l	58	ALA	ASN	engineered mutation	UNP P26535
l	61	LEU	VAL	engineered mutation	UNP P26535
l	176	SER	CYS	engineered mutation	UNP P26535
l	349	LYS	THR	engineered mutation	UNP P26535
l	352	SER	GLY	engineered mutation	UNP P26535
l	357	GLU	ASP	engineered mutation	UNP P26535
m	54	ASN	SER	engineered mutation	UNP P26535
m	56	THR	ASN	engineered mutation	UNP P26535
m	58	ALA	ASN	engineered mutation	UNP P26535
m	61	LEU	VAL	engineered mutation	UNP P26535
m	176	SER	CYS	engineered mutation	UNP P26535
m	349	LYS	THR	engineered mutation	UNP P26535
m	352	SER	GLY	engineered mutation	UNP P26535
m	357	GLU	ASP	engineered mutation	UNP P26535
n	54	ASN	SER	engineered mutation	UNP P26535
n	56	THR	ASN	engineered mutation	UNP P26535
n	58	ALA	ASN	engineered mutation	UNP P26535
n	61	LEU	VAL	engineered mutation	UNP P26535
n	176	SER	CYS	engineered mutation	UNP P26535
n	349	LYS	THR	engineered mutation	UNP P26535
n	352	SER	GLY	engineered mutation	UNP P26535
n	357	GLU	ASP	engineered mutation	UNP P26535

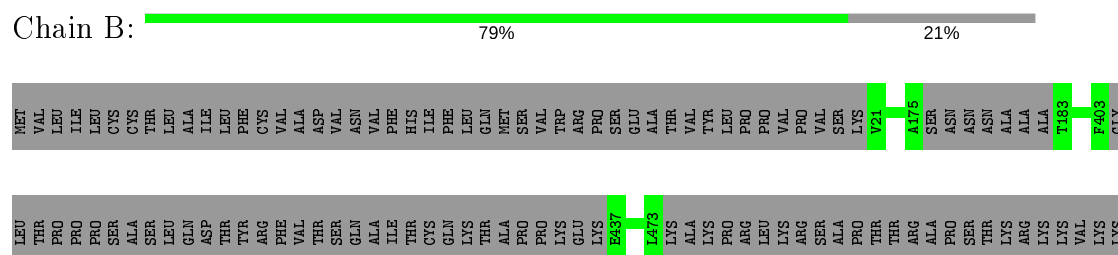
### 3 Residue-property plots

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

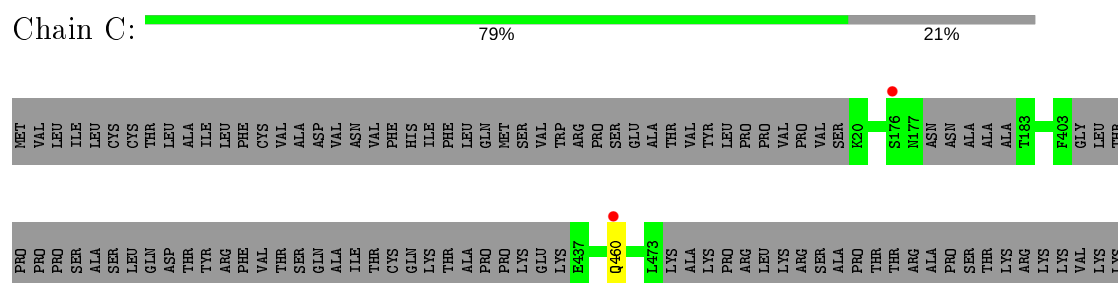
- Molecule 1: Major capsid protein L1



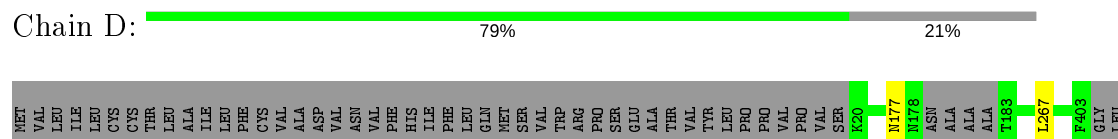
- Molecule 1: Major capsid protein L1

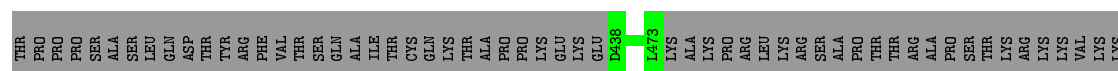


- Molecule 1: Major capsid protein L1

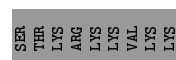
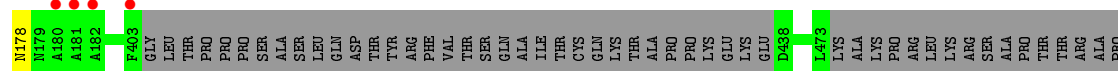
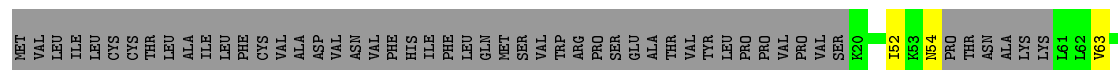
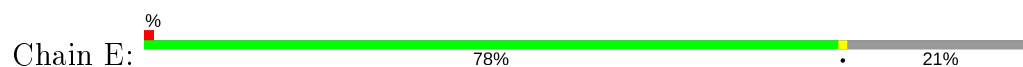


- Molecule 1: Major capsid protein L1

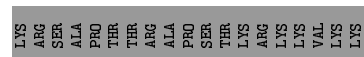
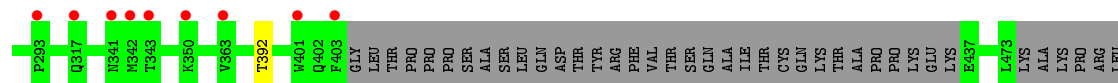
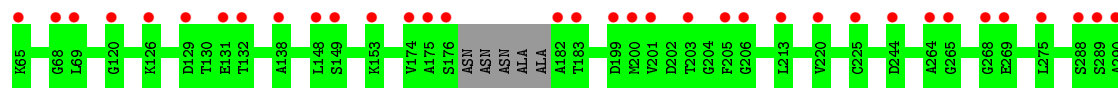
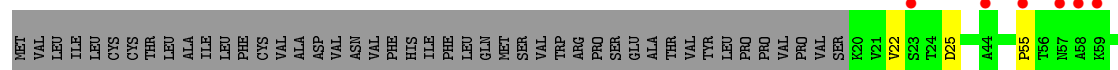
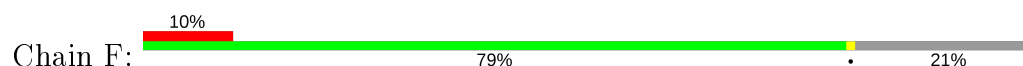




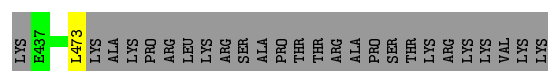
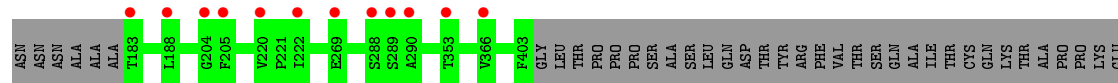
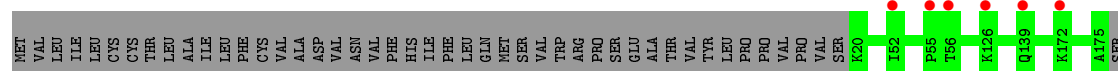
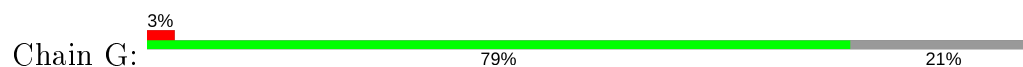
- Molecule 1: Major capsid protein L1



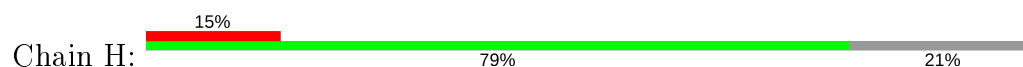
- Molecule 1: Major capsid protein L1



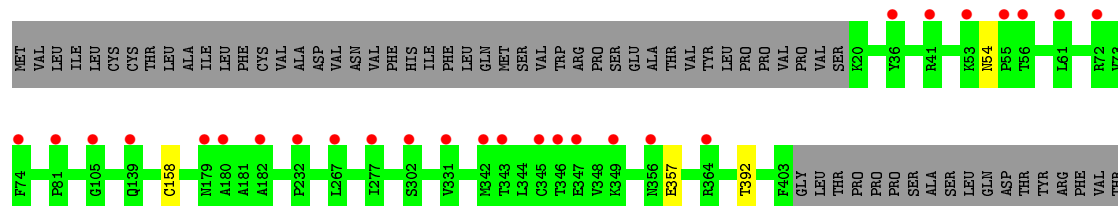
- Molecule 1: Major capsid protein L1

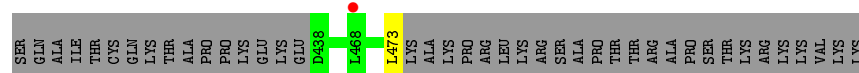


- Molecule 1: Major capsid protein L1

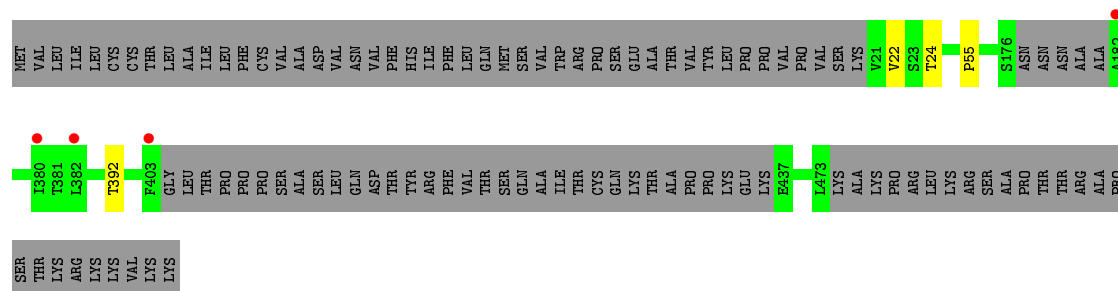
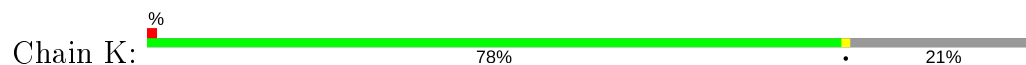




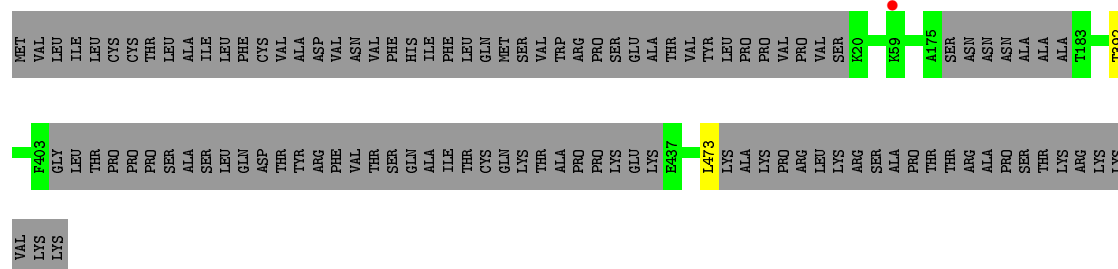
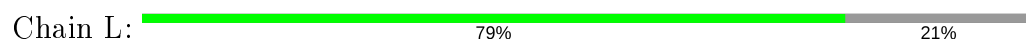




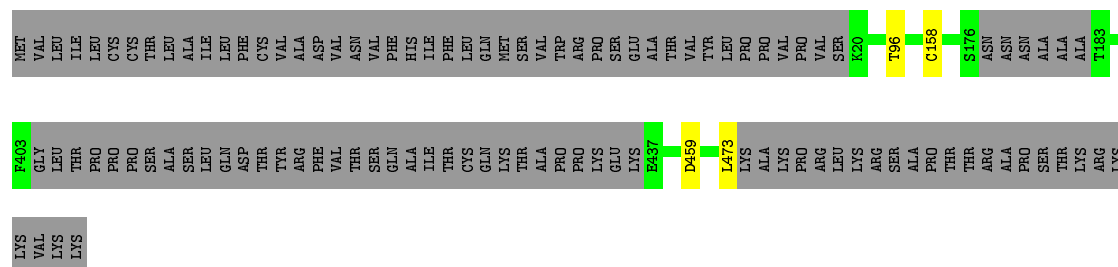
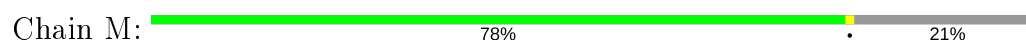
- Molecule 1: Major capsid protein L1



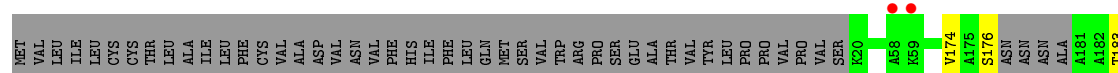
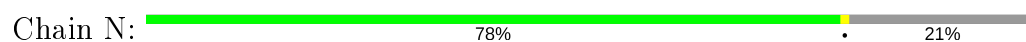
- Molecule 1: Major capsid protein L1

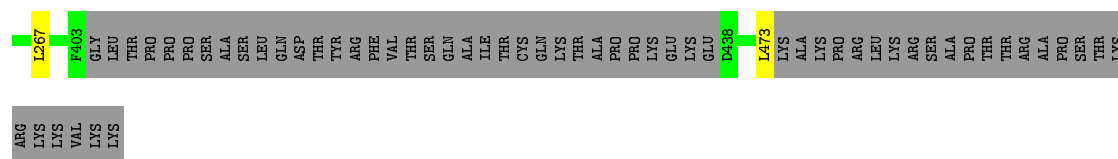


- Molecule 1: Major capsid protein L1

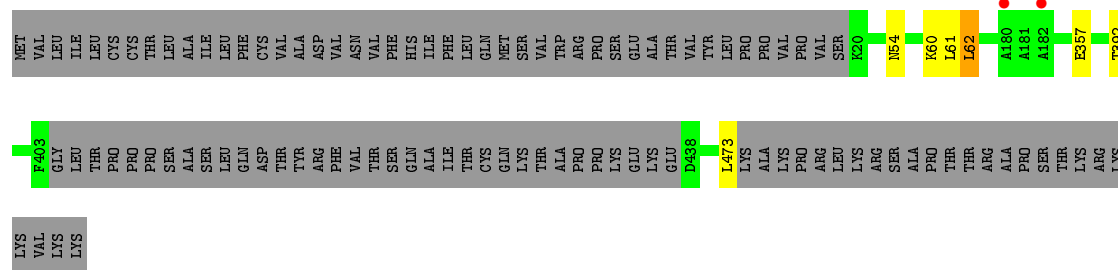
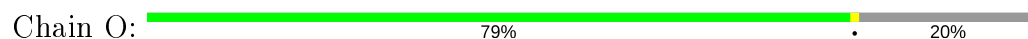


- Molecule 1: Major capsid protein L1

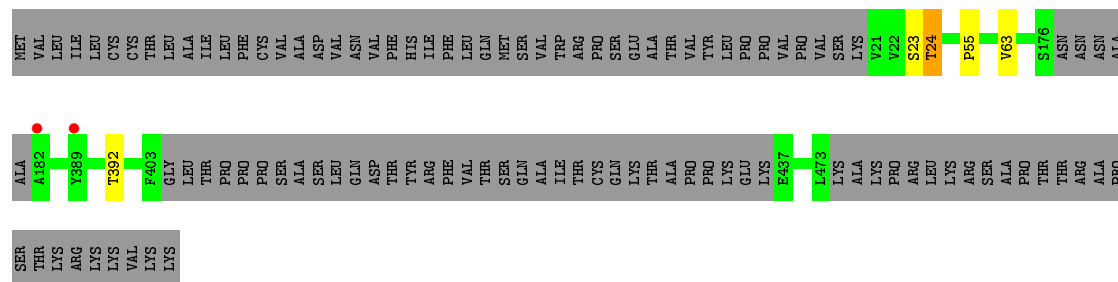
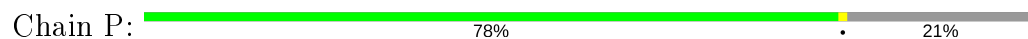




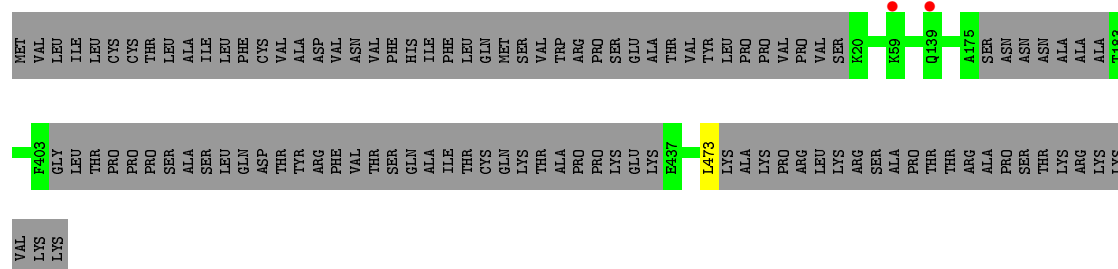
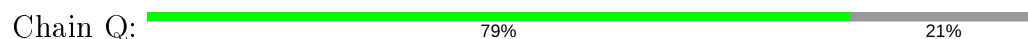
- Molecule 1: Major capsid protein L1



- Molecule 1: Major capsid protein L1

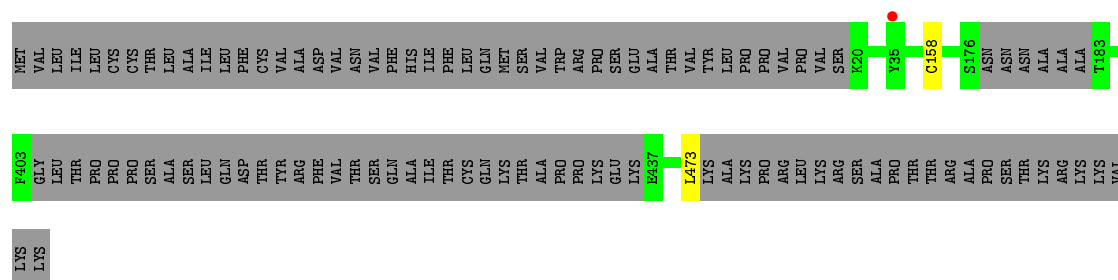


- Molecule 1: Major capsid protein L1

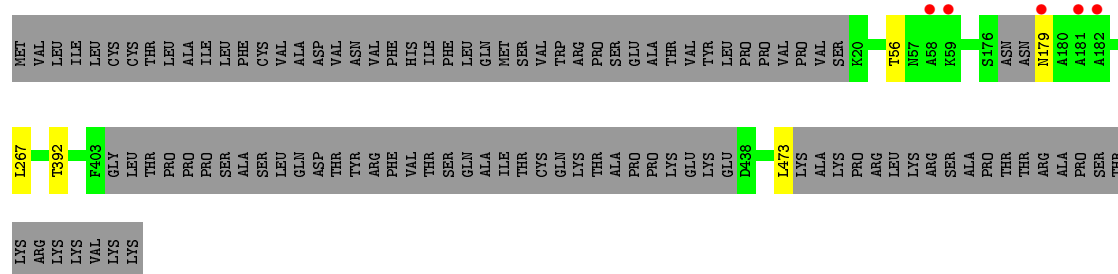
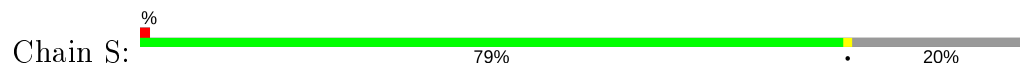


- Molecule 1: Major capsid protein L1

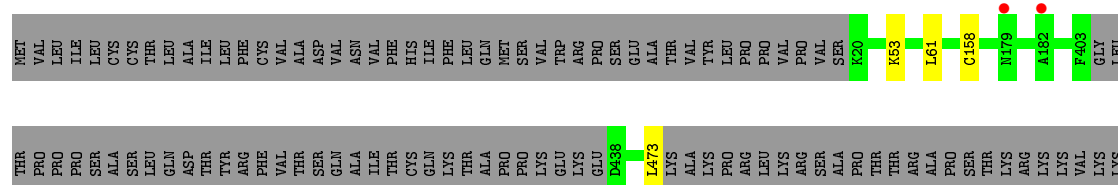
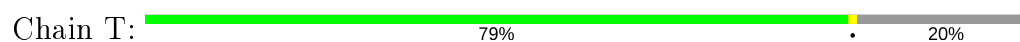




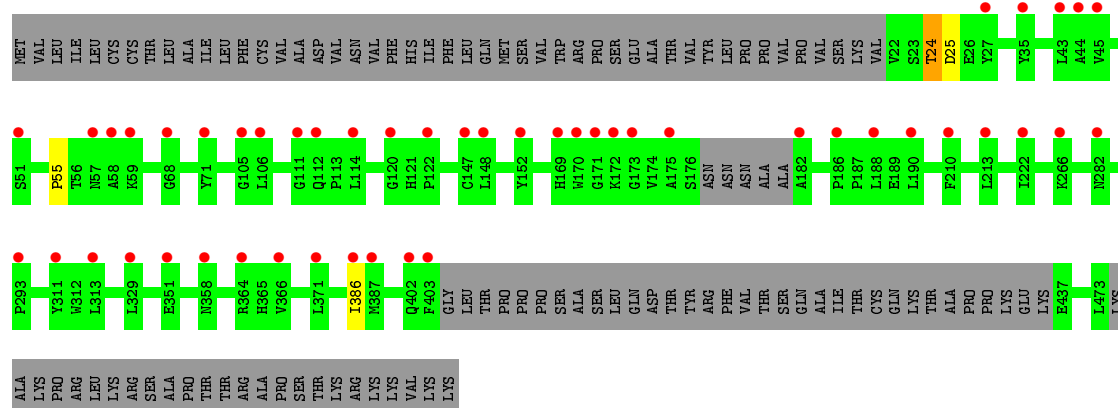
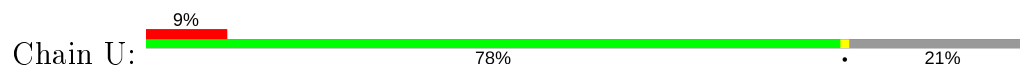
- Molecule 1: Major capsid protein L1



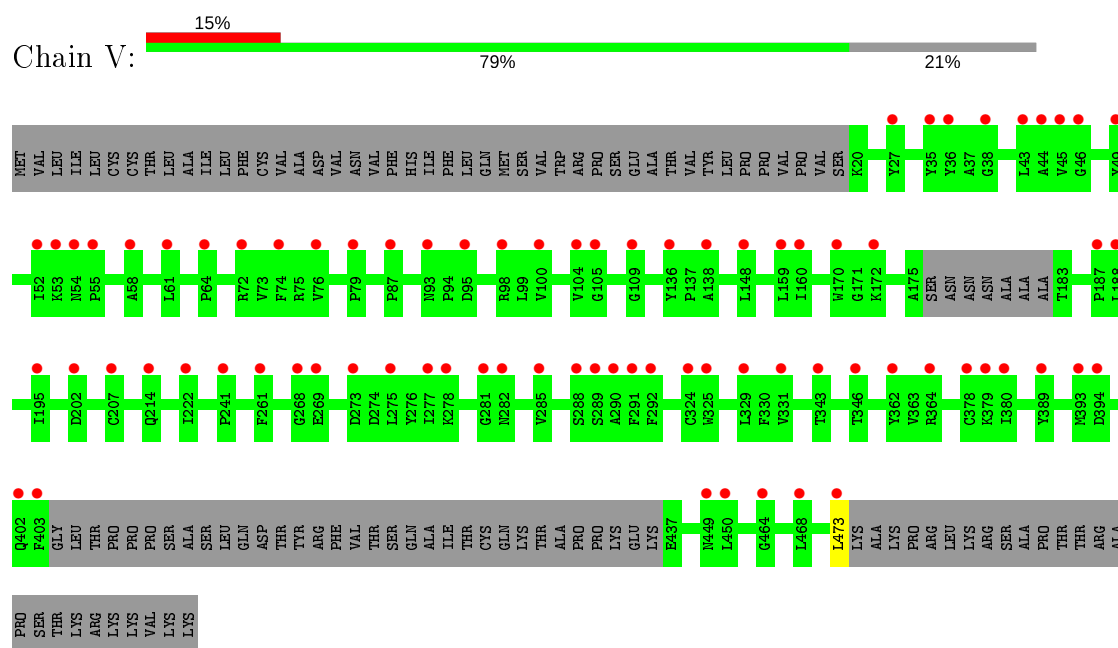
- Molecule 1: Major capsid protein L1



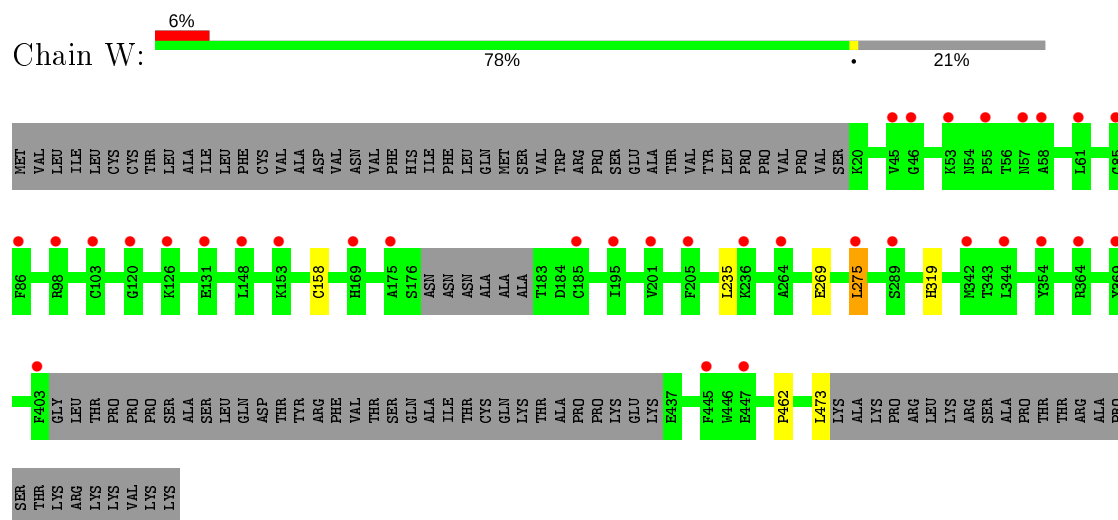
- Molecule 1: Major capsid protein L1



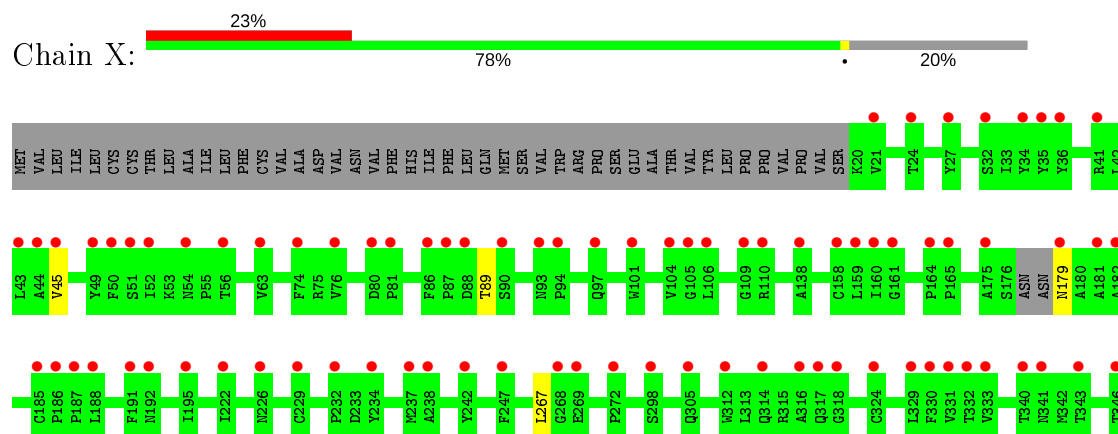
- Molecule 1: Major capsid protein L1

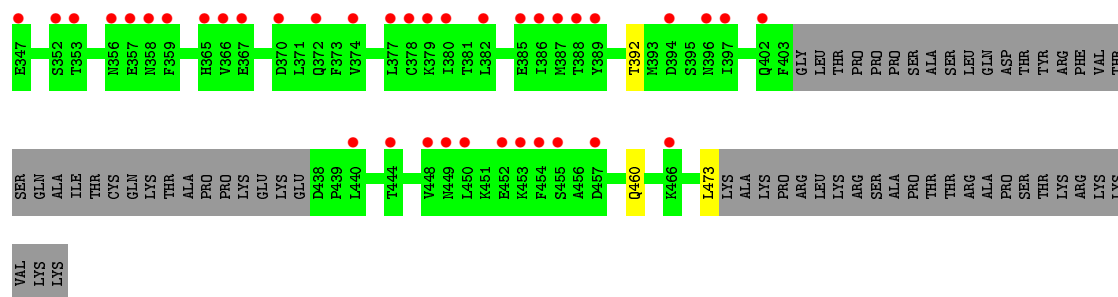


- Molecule 1: Major capsid protein L1

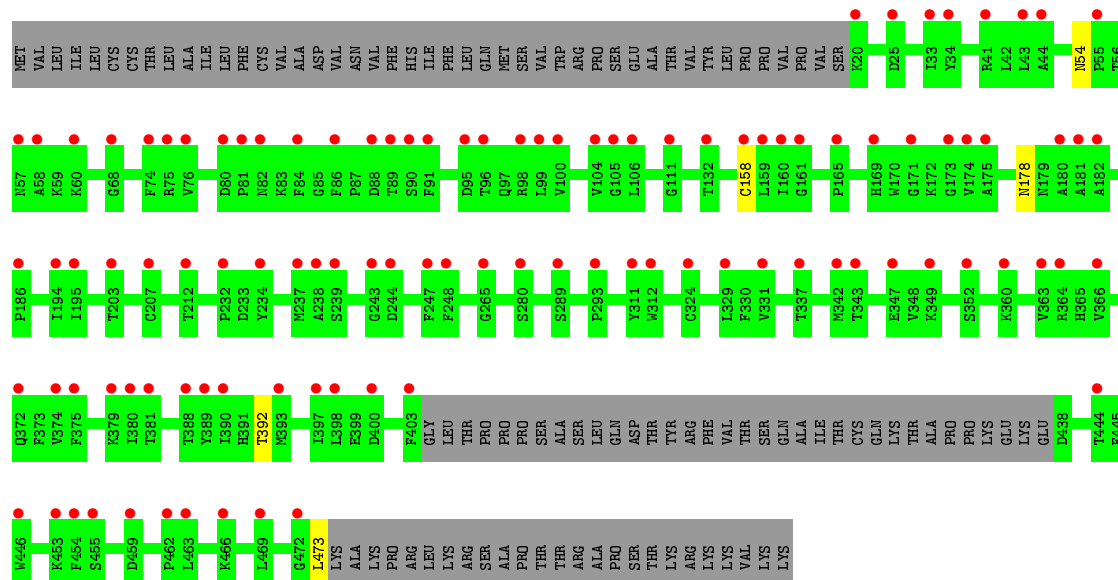
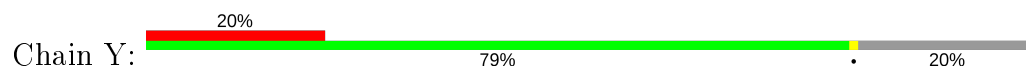


- Molecule 1: Major capsid protein L1

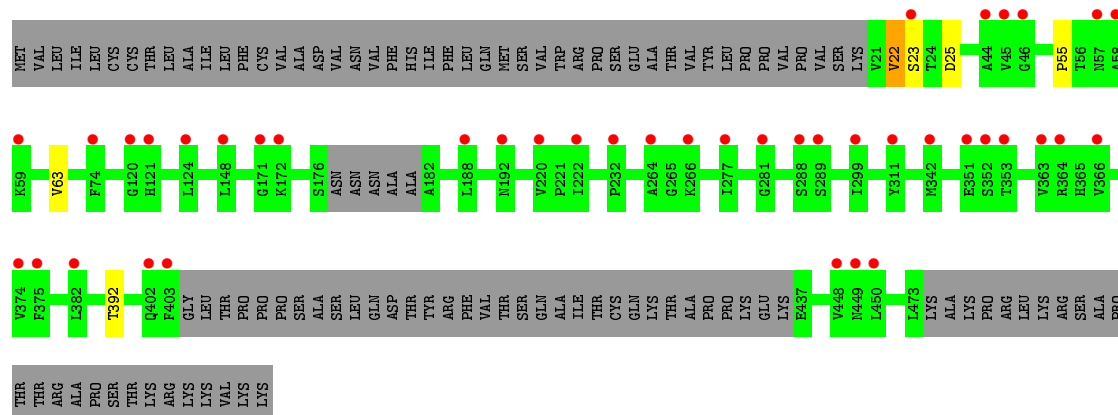
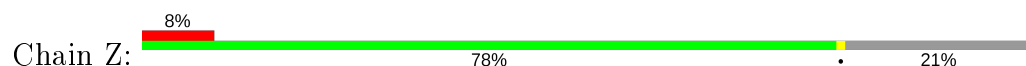




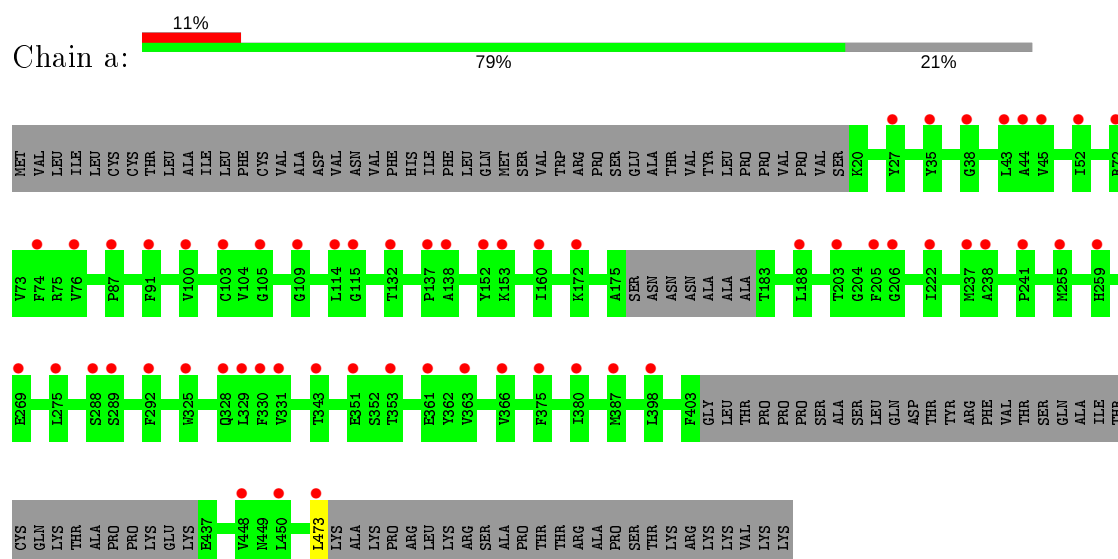
- Molecule 1: Major capsid protein L1



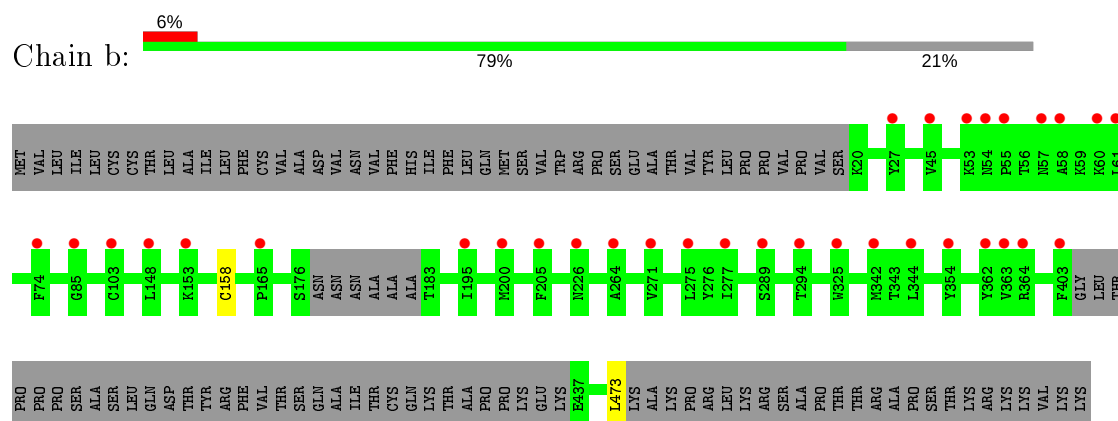
- Molecule 1: Major capsid protein L1



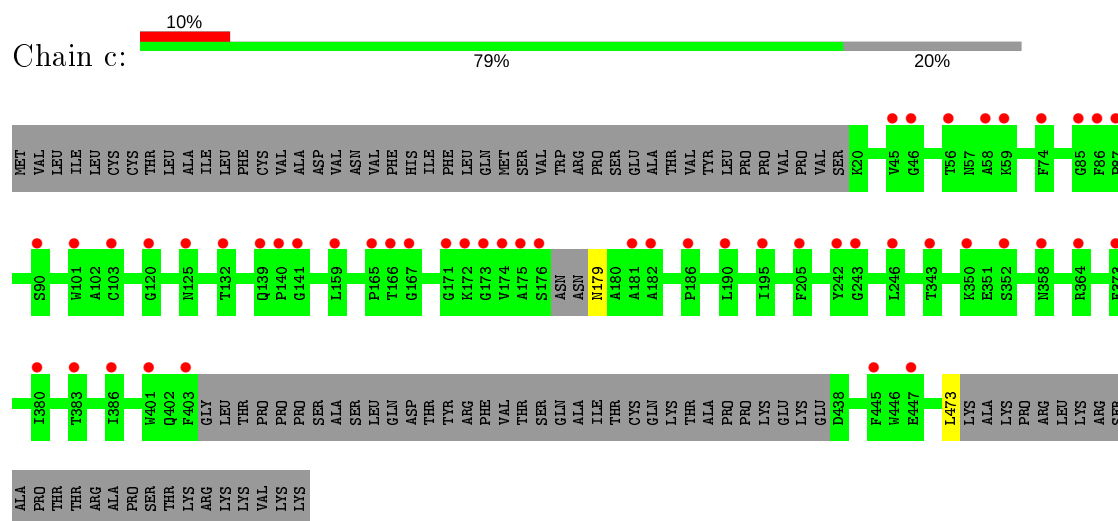
- Molecule 1: Major capsid protein L1



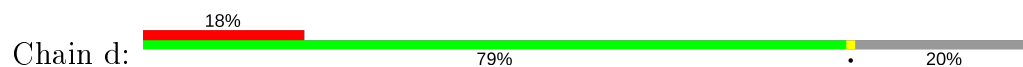
- Molecule 1: Major capsid protein L1

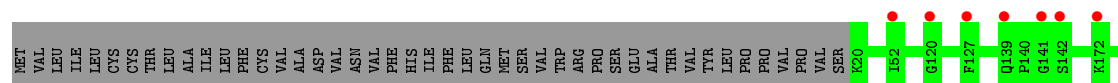


- Molecule 1: Major capsid protein L1



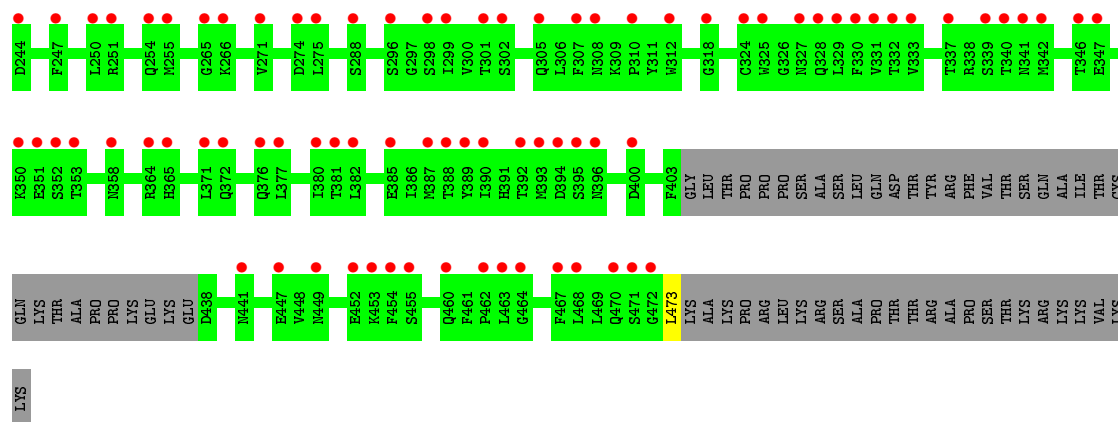
- Molecule 1: Major capsid protein L1



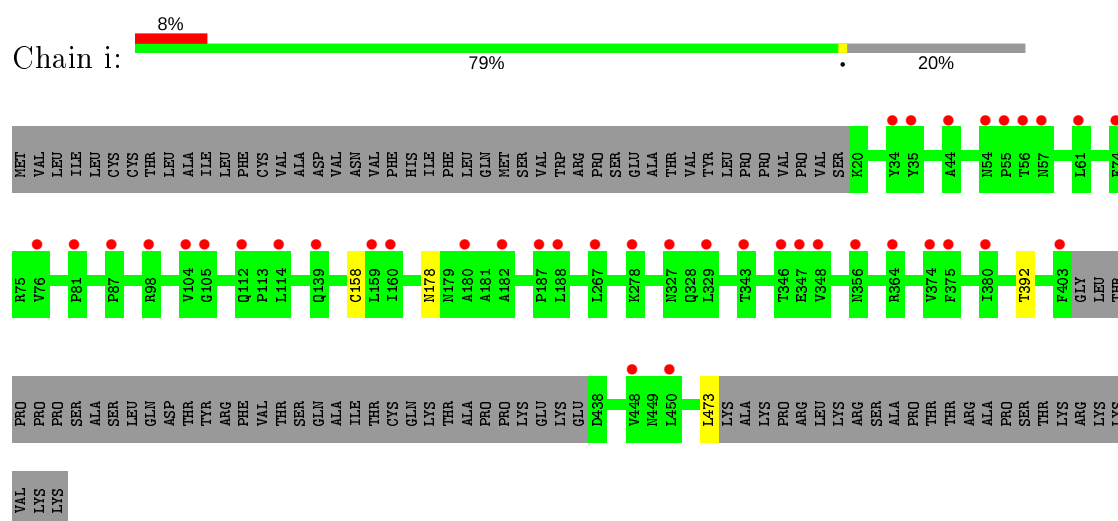




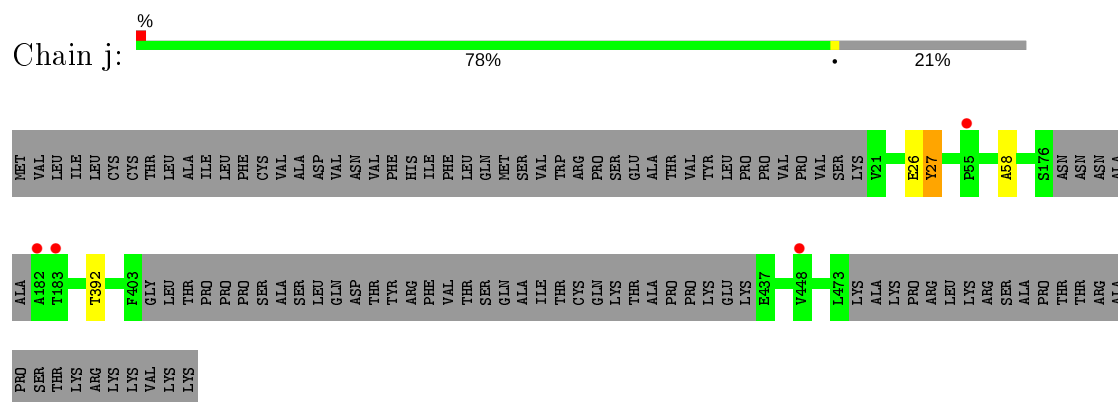




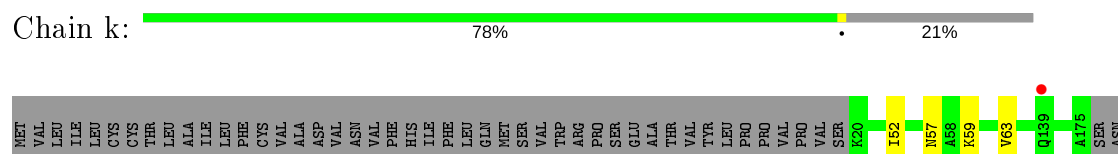
- Molecule 1: Major capsid protein L1

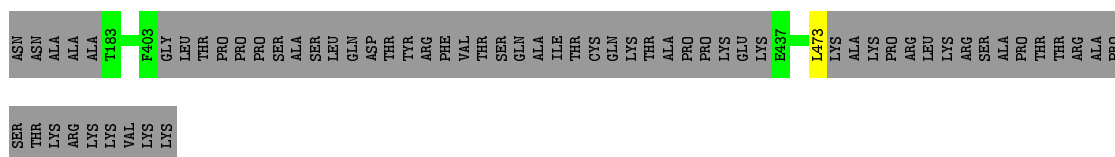


- Molecule 1: Major capsid protein L1

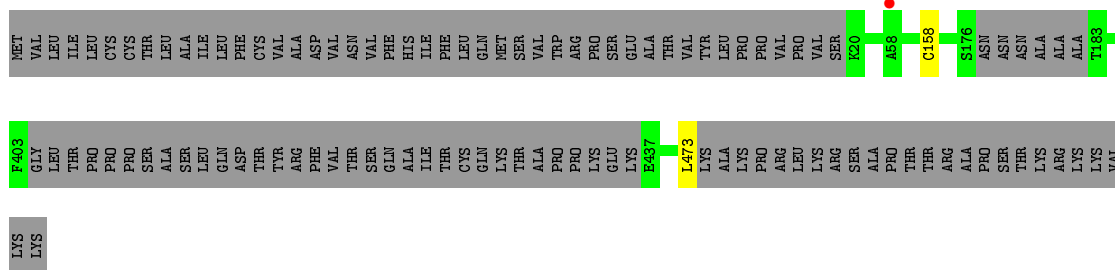
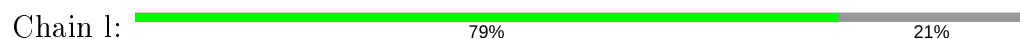


- Molecule 1: Major capsid protein L1

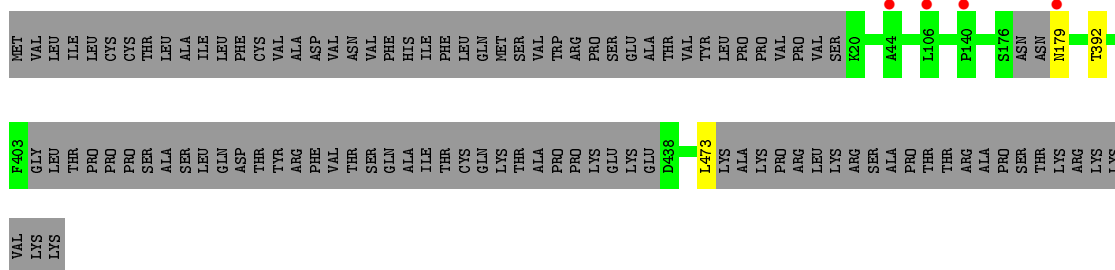
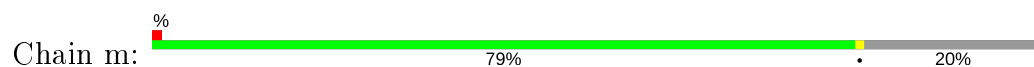




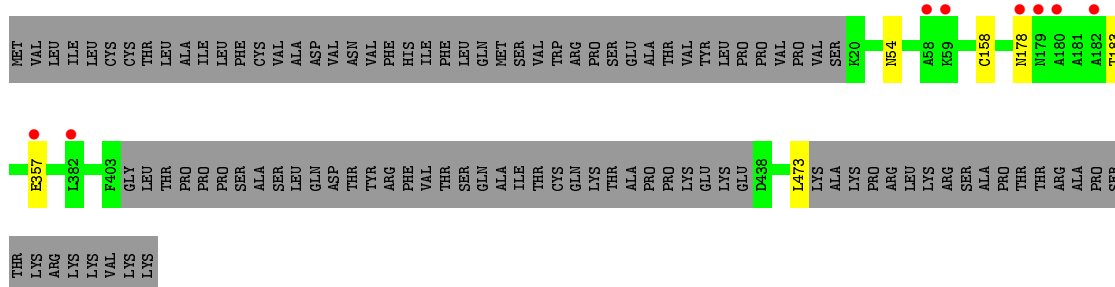
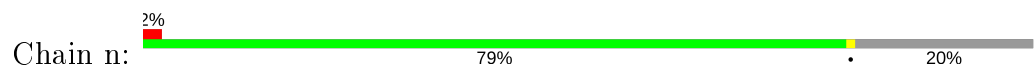
- Molecule 1: Major capsid protein L1



- Molecule 1: Major capsid protein L1



- Molecule 1: Major capsid protein L1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.54Å 209.76Å 212.63Å 60.50° 85.07° 90.12°	Depositor
Resolution (Å)	41.55 – 3.50 41.55 – 3.49	Depositor EDS
% Data completeness (in resolution range)	95.9 (41.55-3.50) 95.8 (41.55-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.315 , 0.340 0.315 , 0.340	Depositor DCC
$R_{free}$ test set	12024 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.6	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 19.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.135 for -h,k,k-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	133128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3375e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	A	0.28	0/3442	0.48	0/4670
1	B	0.26	0/3396	0.46	0/4605
1	C	0.27	0/3413	0.47	1/4627 (0.0%)
1	D	0.27	0/3418	0.47	0/4634
1	E	0.28	0/3395	0.49	2/4604 (0.0%)
1	F	0.26	0/3416	0.46	0/4631
1	G	0.26	0/3405	0.46	0/4616
1	H	0.26	0/3411	0.47	1/4624 (0.0%)
1	I	0.25	0/3425	0.46	0/4644
1	J	0.26	0/3442	0.46	0/4669
1	K	0.27	0/3407	0.48	0/4620
1	L	0.27	0/3405	0.47	0/4616
1	M	0.27	0/3411	0.47	0/4624
1	N	0.27	0/3412	0.47	0/4626
1	O	0.27	0/3442	0.48	1/4669 (0.0%)
1	P	0.26	0/3407	0.48	0/4620
1	Q	0.26	0/3405	0.46	0/4616
1	R	0.26	0/3411	0.48	0/4624
1	S	0.27	0/3425	0.47	0/4644
1	T	0.27	0/3442	0.47	0/4669
1	U	0.26	0/3400	0.46	0/4610
1	V	0.26	0/3405	0.46	0/4616
1	W	0.29	0/3411	0.53	2/4624 (0.0%)
1	X	0.28	0/3425	0.52	0/4644
1	Y	0.26	0/3442	0.47	0/4669
1	Z	0.27	0/3407	0.47	0/4620
1	a	0.26	0/3405	0.46	0/4616
1	b	0.26	0/3411	0.45	0/4624
1	c	0.25	0/3425	0.46	0/4644
1	d	0.25	0/3442	0.46	0/4669
1	e	0.28	0/3416	0.50	0/4631
1	f	0.27	0/3405	0.48	0/4616
1	g	0.26	0/3411	0.47	0/4624
1	h	0.26	0/3425	0.48	0/4644

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	i	0.27	0/3442	0.47	0/4669
1	j	0.27	0/3407	0.47	0/4620
1	k	0.26	0/3405	0.47	0/4616
1	l	0.26	0/3411	0.47	0/4624
1	m	0.26	0/3425	0.47	0/4644
1	n	0.26	0/3442	0.47	0/4669
All	All	0.27	0/136692	0.47	7/185345 (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	j	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	62	LEU	CA-CB-CG	6.37	129.94	115.30
1	C	460	GLN	C-N-CA	-5.64	107.59	121.70
1	W	235	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	E	63	VAL	CG1-CB-CG2	-5.37	102.30	110.90
1	H	460	GLN	C-N-CA	-5.22	108.64	121.70
1	W	275	LEU	CA-CB-CG	5.15	127.14	115.30
1	E	52	ILE	CG1-CB-CG2	-5.07	100.25	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	j	27	TYR	Peptide

## 5.2 Too-close contacts

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	417/524 (80%)	399 (96%)	17 (4%)	1 (0%)	47	81
1	B	408/524 (78%)	389 (95%)	19 (5%)	0	100	100
1	C	410/524 (78%)	392 (96%)	18 (4%)	0	100	100
1	D	411/524 (78%)	392 (95%)	19 (5%)	0	100	100
1	E	409/524 (78%)	391 (96%)	17 (4%)	1 (0%)	47	81
1	F	411/524 (78%)	388 (94%)	20 (5%)	3 (1%)	22	61
1	G	409/524 (78%)	391 (96%)	18 (4%)	0	100	100
1	H	410/524 (78%)	391 (95%)	19 (5%)	0	100	100
1	I	413/524 (79%)	394 (95%)	19 (5%)	0	100	100
1	J	417/524 (80%)	398 (95%)	19 (5%)	0	100	100
1	K	410/524 (78%)	392 (96%)	16 (4%)	2 (0%)	29	68
1	L	409/524 (78%)	391 (96%)	18 (4%)	0	100	100
1	M	410/524 (78%)	393 (96%)	17 (4%)	0	100	100
1	N	411/524 (78%)	392 (95%)	19 (5%)	0	100	100
1	O	417/524 (80%)	400 (96%)	17 (4%)	0	100	100
1	P	410/524 (78%)	390 (95%)	18 (4%)	2 (0%)	29	68
1	Q	409/524 (78%)	391 (96%)	18 (4%)	0	100	100
1	R	410/524 (78%)	391 (95%)	19 (5%)	0	100	100
1	S	413/524 (79%)	393 (95%)	20 (5%)	0	100	100
1	T	417/524 (80%)	401 (96%)	16 (4%)	0	100	100
1	U	409/524 (78%)	390 (95%)	17 (4%)	2 (0%)	29	68
1	V	409/524 (78%)	390 (95%)	19 (5%)	0	100	100
1	W	410/524 (78%)	392 (96%)	17 (4%)	1 (0%)	47	81
1	X	413/524 (79%)	394 (95%)	19 (5%)	0	100	100
1	Y	417/524 (80%)	399 (96%)	17 (4%)	1 (0%)	47	81

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	410/524 (78%)	389 (95%)	17 (4%)	4 (1%)	15	54
1	a	409/524 (78%)	389 (95%)	20 (5%)	0	100	100
1	b	410/524 (78%)	392 (96%)	18 (4%)	0	100	100
1	c	413/524 (79%)	395 (96%)	18 (4%)	0	100	100
1	d	417/524 (80%)	399 (96%)	18 (4%)	0	100	100
1	e	411/524 (78%)	388 (94%)	19 (5%)	4 (1%)	15	54
1	f	409/524 (78%)	389 (95%)	20 (5%)	0	100	100
1	g	410/524 (78%)	393 (96%)	17 (4%)	0	100	100
1	h	413/524 (79%)	395 (96%)	18 (4%)	0	100	100
1	i	417/524 (80%)	397 (95%)	19 (5%)	1 (0%)	47	81
1	j	410/524 (78%)	390 (95%)	19 (5%)	1 (0%)	47	81
1	k	409/524 (78%)	391 (96%)	18 (4%)	0	100	100
1	l	410/524 (78%)	391 (95%)	19 (5%)	0	100	100
1	m	413/524 (79%)	395 (96%)	18 (4%)	0	100	100
1	n	417/524 (80%)	397 (95%)	19 (5%)	1 (0%)	47	81
All	All	16467/20960 (79%)	15714 (95%)	729 (4%)	24 (0%)	51	84

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	PRO
1	F	25	ASP
1	P	24	THR
1	Z	25	ASP
1	e	25	ASP
1	e	22	VAL
1	e	23	SER
1	n	178	ASN
1	E	178	ASN
1	K	22	VAL
1	Z	23	SER
1	i	178	ASN
1	U	24	THR
1	W	462	PRO
1	Y	178	ASN
1	j	58	ALA
1	Z	22	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	22	VAL
1	F	55	PRO
1	K	55	PRO
1	P	55	PRO
1	U	55	PRO
1	Z	55	PRO
1	e	55	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	373/466 (80%)	369 (99%)	4 (1%)	73	88
1	B	369/466 (79%)	369 (100%)	0	100	100
1	C	371/466 (80%)	371 (100%)	0	100	100
1	D	372/466 (80%)	370 (100%)	2 (0%)	88	94
1	E	368/466 (79%)	367 (100%)	1 (0%)	92	97
1	F	371/466 (80%)	370 (100%)	1 (0%)	92	97
1	G	370/466 (79%)	369 (100%)	1 (0%)	92	97
1	H	371/466 (80%)	367 (99%)	4 (1%)	73	88
1	I	371/466 (80%)	367 (99%)	4 (1%)	73	88
1	J	373/466 (80%)	367 (98%)	6 (2%)	62	83
1	K	370/466 (79%)	368 (100%)	2 (0%)	88	94
1	L	370/466 (79%)	368 (100%)	2 (0%)	88	94
1	M	371/466 (80%)	366 (99%)	5 (1%)	69	86
1	N	370/466 (79%)	365 (99%)	5 (1%)	67	85
1	O	373/466 (80%)	366 (98%)	7 (2%)	57	80
1	P	370/466 (79%)	366 (99%)	4 (1%)	73	88
1	Q	370/466 (79%)	369 (100%)	1 (0%)	92	97
1	R	371/466 (80%)	368 (99%)	3 (1%)	81	91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	371/466 (80%)	366 (99%)	5 (1%)	69	86
1	T	373/466 (80%)	368 (99%)	5 (1%)	69	86
1	U	369/466 (79%)	366 (99%)	3 (1%)	81	91
1	V	370/466 (79%)	369 (100%)	1 (0%)	92	97
1	W	371/466 (80%)	365 (98%)	6 (2%)	62	83
1	X	371/466 (80%)	365 (98%)	6 (2%)	62	83
1	Y	373/466 (80%)	368 (99%)	5 (1%)	69	86
1	Z	370/466 (79%)	367 (99%)	3 (1%)	81	91
1	a	370/466 (79%)	369 (100%)	1 (0%)	92	97
1	b	371/466 (80%)	368 (99%)	3 (1%)	81	91
1	c	371/466 (80%)	369 (100%)	2 (0%)	88	94
1	d	373/466 (80%)	368 (99%)	5 (1%)	69	86
1	e	371/466 (80%)	368 (99%)	3 (1%)	81	91
1	f	370/466 (79%)	368 (100%)	2 (0%)	88	94
1	g	371/466 (80%)	367 (99%)	4 (1%)	73	88
1	h	371/466 (80%)	368 (99%)	3 (1%)	81	91
1	i	373/466 (80%)	369 (99%)	4 (1%)	73	88
1	j	370/466 (79%)	367 (99%)	3 (1%)	81	91
1	k	370/466 (79%)	365 (99%)	5 (1%)	67	85
1	l	371/466 (80%)	368 (99%)	3 (1%)	81	91
1	m	371/466 (80%)	368 (99%)	3 (1%)	81	91
1	n	373/466 (80%)	367 (98%)	6 (2%)	62	83
All	All	14838/18640 (80%)	14705 (99%)	133 (1%)	81	90

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	177	ASN
1	A	178	ASN
1	A	183	THR
1	D	177	ASN
1	D	267	LEU
1	E	54	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	392	THR
1	G	473	LEU
1	H	158[A]	CYS
1	H	158[B]	CYS
1	H	460	GLN
1	H	473	LEU
1	I	179	ASN
1	I	267	LEU
1	I	392	THR
1	I	473	LEU
1	J	54	ASN
1	J	158[A]	CYS
1	J	158[B]	CYS
1	J	357	GLU
1	J	392	THR
1	J	473	LEU
1	K	24	THR
1	K	392	THR
1	L	392	THR
1	L	473	LEU
1	M	96	THR
1	M	158[A]	CYS
1	M	158[B]	CYS
1	M	459	ASP
1	M	473	LEU
1	N	174	VAL
1	N	176	SER
1	N	183	THR
1	N	267	LEU
1	N	473	LEU
1	O	54	ASN
1	O	60	LYS
1	O	61	LEU
1	O	62	LEU
1	O	357	GLU
1	O	392	THR
1	O	473	LEU
1	P	23	SER
1	P	24	THR
1	P	63	VAL
1	P	392	THR
1	Q	473	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	R	158[A]	CYS
1	R	158[B]	CYS
1	R	473	LEU
1	S	56	THR
1	S	179	ASN
1	S	267	LEU
1	S	392	THR
1	S	473	LEU
1	T	53	LYS
1	T	61	LEU
1	T	158[A]	CYS
1	T	158[B]	CYS
1	T	473	LEU
1	U	24	THR
1	U	25	ASP
1	U	386	ILE
1	V	473	LEU
1	W	158[A]	CYS
1	W	158[B]	CYS
1	W	269	GLU
1	W	275	LEU
1	W	319	HIS
1	W	473	LEU
1	X	45	VAL
1	X	179	ASN
1	X	267	LEU
1	X	392	THR
1	X	460	GLN
1	X	473	LEU
1	Y	54	ASN
1	Y	158[A]	CYS
1	Y	158[B]	CYS
1	Y	392	THR
1	Y	473	LEU
1	Z	22	VAL
1	Z	63	VAL
1	Z	392	THR
1	a	473	LEU
1	b	158[A]	CYS
1	b	158[B]	CYS
1	b	473	LEU
1	c	179	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	c	473	LEU
1	d	54	ASN
1	d	158[A]	CYS
1	d	158[B]	CYS
1	d	357	GLU
1	d	473	LEU
1	e	21	VAL
1	e	217	LYS
1	e	225	CYS
1	f	277	ILE
1	f	473	LEU
1	g	158[A]	CYS
1	g	158[B]	CYS
1	g	460	GLN
1	g	473	LEU
1	h	158[A]	CYS
1	h	158[B]	CYS
1	h	473	LEU
1	i	158[A]	CYS
1	i	158[B]	CYS
1	i	392	THR
1	i	473	LEU
1	j	26	GLU
1	j	27	TYR
1	j	392	THR
1	k	52	ILE
1	k	57	ASN
1	k	59	LYS
1	k	63	VAL
1	k	473	LEU
1	l	158[A]	CYS
1	l	158[B]	CYS
1	l	473	LEU
1	m	179	ASN
1	m	392	THR
1	m	473	LEU
1	n	54	ASN
1	n	158[A]	CYS
1	n	158[B]	CYS
1	n	183	THR
1	n	357	GLU
1	n	473	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	B	154	GLN
1	B	282	ASN
1	C	356	ASN
1	E	54	ASN
1	E	154	GLN
1	E	254	GLN
1	F	139	GLN
1	F	314	GLN
1	G	154	GLN
1	J	356	ASN
1	K	314	GLN
1	L	154	GLN
1	M	460	GLN
1	O	356	ASN
1	Q	154	GLN
1	R	154	GLN
1	R	460	GLN
1	T	57	ASN
1	U	139	GLN
1	U	254	GLN
1	V	154	GLN
1	V	282	ASN
1	W	356	ASN
1	Y	282	ASN
1	Y	356	ASN
1	Z	139	GLN
1	Z	154	GLN
1	Z	254	GLN
1	Z	314	GLN
1	a	154	GLN
1	b	139	GLN
1	d	282	ASN
1	d	356	ASN
1	f	154	GLN
1	g	327	ASN
1	g	460	GLN
1	i	112	GLN
1	k	57	ASN
1	k	154	GLN
1	k	282	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	l	254	GLN
1	m	254	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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	420/524 (80%)	-0.27	1 (0%) 95 93	27, 48, 99, 169	0
1	B	413/524 (78%)	-0.30	0 100 100	31, 49, 90, 149	0
1	C	416/524 (79%)	-0.24	2 (0%) 91 88	34, 58, 102, 156	0
1	D	416/524 (79%)	-0.21	0 100 100	31, 52, 91, 154	0
1	E	414/524 (79%)	-0.12	4 (0%) 82 77	35, 57, 94, 177	0
1	F	416/524 (79%)	0.63	50 (12%) 4 5	90, 120, 165, 282	0
1	G	414/524 (79%)	0.18	18 (4%) 35 31	82, 105, 154, 200	0
1	H	415/524 (79%)	0.92	79 (19%) 1 1	107, 148, 186, 252	0
1	I	418/524 (79%)	1.08	87 (20%) 1 1	124, 163, 204, 283	0
1	J	420/524 (80%)	0.42	28 (6%) 17 16	98, 136, 180, 339	0
1	K	415/524 (79%)	-0.15	4 (0%) 82 77	26, 50, 91, 204	0
1	L	414/524 (79%)	-0.30	1 (0%) 95 93	22, 48, 101, 157	0
1	M	415/524 (79%)	-0.27	0 100 100	24, 44, 81, 164	0
1	N	416/524 (79%)	-0.23	2 (0%) 91 88	28, 51, 97, 218	0
1	O	420/524 (80%)	-0.27	2 (0%) 91 88	23, 46, 90, 171	0
1	P	415/524 (79%)	-0.02	2 (0%) 91 88	75, 93, 131, 186	0
1	Q	414/524 (79%)	-0.06	2 (0%) 91 88	74, 90, 133, 205	0
1	R	415/524 (79%)	-0.02	1 (0%) 95 93	66, 92, 120, 198	0
1	S	418/524 (79%)	-0.10	5 (1%) 79 73	63, 76, 119, 226	0
1	T	420/524 (80%)	-0.10	2 (0%) 91 88	57, 77, 105, 180	0
1	U	414/524 (79%)	0.61	49 (11%) 4 5	114, 151, 186, 304	0
1	V	414/524 (79%)	0.95	79 (19%) 1 1	81, 149, 192, 215	0
1	W	415/524 (79%)	0.51	34 (8%) 11 12	107, 139, 189, 260	0
1	X	418/524 (79%)	1.66	120 (28%) 0 0	84, 148, 189, 242	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	420/524 (80%)	1.44	106 (25%) 0 0	76, 122, 161, 378	0
1	Z	415/524 (79%)	0.56	42 (10%) 7 7	114, 146, 184, 281	0
1	a	414/524 (79%)	0.72	58 (14%) 2 3	129, 152, 178, 196	0
1	b	415/524 (79%)	0.54	33 (7%) 12 12	105, 148, 177, 270	0
1	c	418/524 (79%)	0.71	50 (11%) 4 5	113, 146, 182, 291	0
1	d	420/524 (80%)	1.10	92 (21%) 0 0	114, 159, 202, 390	0
1	e	416/524 (79%)	2.17	158 (37%) 0 0	73, 126, 167, 256	0
1	f	414/524 (79%)	0.29	26 (6%) 20 18	39, 85, 168, 212	0
1	g	415/524 (79%)	2.38	177 (42%) 0 0	100, 126, 156, 226	0
1	h	418/524 (79%)	2.13	173 (41%) 0 0	89, 123, 167, 227	0
1	i	420/524 (80%)	0.53	40 (9%) 8 8	68, 132, 185, 335	0
1	j	415/524 (79%)	-0.13	4 (0%) 82 77	50, 72, 109, 166	0
1	k	414/524 (79%)	-0.13	1 (0%) 95 93	63, 82, 118, 172	0
1	l	415/524 (79%)	-0.13	1 (0%) 95 93	69, 82, 124, 221	0
1	m	418/524 (79%)	-0.12	4 (0%) 82 77	63, 82, 116, 194	0
1	n	420/524 (80%)	-0.03	8 (1%) 66 61	58, 81, 132, 351	0
All	All	16652/20960 (79%)	0.41	1545 (9%) 8 9	22, 103, 174, 390	0

All (1545) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	e	165	PRO	18.1
1	g	119	SER	16.9
1	g	247	PHE	16.9
1	g	158[A]	CYS	16.4
1	X	105	GLY	14.3
1	e	24	THR	13.8
1	Y	160	ILE	13.6
1	g	160	ILE	13.1
1	e	176	SER	12.6
1	Y	105	GLY	12.4
1	e	46	GLY	12.1
1	h	330	PHE	11.9
1	Y	381	THR	11.8
1	Y	161	GLY	11.8
1	g	264	ALA	11.8

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	d	58	ALA	11.7
1	X	44	ALA	11.6
1	e	173	GLY	11.6
1	Z	403	PHE	11.4
1	e	316	ALA	11.4
1	e	386	ILE	11.4
1	X	389	TYR	11.2
1	h	161	GLY	11.0
1	h	390	ILE	10.9
1	Y	181	ALA	10.8
1	h	380	ILE	10.7
1	H	175	ALA	10.5
1	g	233	ASP	10.2
1	g	173	GLY	10.1
1	h	202	ASP	10.1
1	e	44	ALA	10.0
1	h	53	LYS	10.0
1	h	389	TYR	9.8
1	h	179	ASN	9.4
1	f	289	SER	9.3
1	X	179	ASN	9.3
1	X	331	VAL	9.2
1	d	181	ALA	9.2
1	h	233	ASP	9.0
1	X	455	SER	9.0
1	h	327	ASN	9.0
1	X	352	SER	9.0
1	h	395	SER	9.0
1	X	45	VAL	8.9
1	g	331	VAL	8.9
1	g	151	ASP	8.9
1	X	24	THR	8.9
1	h	381	THR	8.9
1	h	394	ASP	8.9
1	h	89	THR	8.9
1	d	99	LEU	8.9
1	h	332	THR	8.8
1	X	186	PRO	8.7
1	g	226	ASN	8.7
1	e	382	LEU	8.7
1	e	287	GLN	8.6
1	g	437	GLU	8.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	g	29	SER	8.5
1	f	288	SER	8.5
1	e	261	PHE	8.4
1	Y	329	LEU	8.4
1	X	86	PHE	8.4
1	g	234	TYR	8.4
1	g	232	PRO	8.3
1	g	161	GLY	8.3
1	e	290	ALA	8.2
1	Y	342	MET	8.1
1	Y	88	ASP	8.1
1	h	232	PRO	8.1
1	e	57	ASN	8.0
1	e	281	GLY	8.0
1	e	284	ALA	8.0
1	F	289	SER	8.0
1	X	109	GLY	7.9
1	X	187	PRO	7.9
1	H	192	ASN	7.9
1	d	182	ALA	7.9
1	h	46	GLY	7.9
1	i	346	THR	7.8
1	h	117	GLY	7.8
1	g	203	THR	7.7
1	g	55	PRO	7.7
1	X	165	PRO	7.6
1	e	164	PRO	7.6
1	Y	247	PHE	7.6
1	h	159	LEU	7.6
1	g	378	CYS	7.6
1	c	140	PRO	7.5
1	g	248	PHE	7.5
1	e	185	CYS	7.5
1	f	290	ALA	7.5
1	h	329	LEU	7.5
1	d	57	ASN	7.5
1	e	317	GLN	7.4
1	h	186	PRO	7.4
1	F	58	ALA	7.4
1	e	377	LEU	7.4
1	g	276	TYR	7.4
1	e	282	ASN	7.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	181	ALA	7.3
1	Z	366	VAL	7.3
1	Y	403	PHE	7.3
1	g	275	LEU	7.2
1	F	59	LYS	7.2
1	d	59	LYS	7.2
1	e	286	ILE	7.1
1	Y	469	LEU	7.1
1	g	100	VAL	7.1
1	g	50	PHE	7.1
1	b	58	ALA	7.0
1	e	203	THR	7.0
1	g	62	LEU	7.0
1	X	387	MET	7.0
1	S	58	ALA	7.0
1	X	453	LYS	7.0
1	U	58	ALA	6.9
1	Y	374	VAL	6.9
1	g	365	HIS	6.9
1	e	383	THR	6.9
1	h	90	SER	6.8
1	X	104	VAL	6.8
1	g	23	SER	6.8
1	O	182	ALA	6.8
1	G	353	THR	6.8
1	Y	104	VAL	6.8
1	Y	331	VAL	6.8
1	V	288	SER	6.8
1	g	265	GLY	6.7
1	g	46	GLY	6.7
1	g	159	LEU	6.7
1	e	184	ASP	6.7
1	I	379	LYS	6.6
1	e	191	PHE	6.6
1	F	57	ASN	6.6
1	e	175	ALA	6.6
1	g	334	VAL	6.6
1	j	182	ALA	6.6
1	I	170	TRP	6.6
1	Z	45	VAL	6.6
1	e	101	TRP	6.6
1	m	179	ASN	6.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	b	55	PRO	6.6
1	X	396	ASN	6.6
1	h	54	ASN	6.5
1	U	403	PHE	6.5
1	g	72	ARG	6.5
1	e	378	CYS	6.5
1	h	34	TYR	6.5
1	X	397	ILE	6.5
1	H	90	SER	6.5
1	T	182	ALA	6.4
1	g	317	GLN	6.4
1	h	109	GLY	6.4
1	Y	99	LEU	6.4
1	Y	80	ASP	6.4
1	g	121	HIS	6.4
1	F	182	ALA	6.4
1	h	324	CYS	6.4
1	I	58	ALA	6.4
1	h	462	PRO	6.4
1	H	174	VAL	6.4
1	e	172	LYS	6.3
1	N	58	ALA	6.3
1	Y	234	TYR	6.3
1	g	332	THR	6.3
1	i	55	PRO	6.3
1	U	57	ASN	6.3
1	h	376	GLN	6.3
1	h	201	VAL	6.2
1	Z	352	SER	6.2
1	h	222	ILE	6.2
1	e	388	THR	6.2
1	h	88	ASP	6.2
1	H	116	VAL	6.2
1	X	164	PRO	6.1
1	g	22	VAL	6.1
1	I	179	ASN	6.1
1	F	148	LEU	6.1
1	e	205	PHE	6.1
1	d	380	ILE	6.1
1	X	43	LEU	6.0
1	g	399	GLU	6.0
1	H	165	PRO	6.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	X	353	THR	6.0
1	g	324	CYS	6.0
1	e	174	VAL	6.0
1	g	312	TRP	6.0
1	X	332	THR	5.9
1	h	160	ILE	5.9
1	X	160	ILE	5.9
1	g	292	PHE	5.9
1	h	396	ASN	5.8
1	d	100	VAL	5.8
1	H	205	PHE	5.8
1	X	238	ALA	5.8
1	e	285	VAL	5.8
1	I	311	TYR	5.8
1	e	280	SER	5.8
1	d	381	THR	5.8
1	g	389	TYR	5.8
1	Y	180	ALA	5.8
1	X	347	GLU	5.8
1	X	185	CYS	5.8
1	h	227	SER	5.8
1	c	172	LYS	5.8
1	e	45	VAL	5.8
1	X	182	ALA	5.8
1	f	264	ALA	5.7
1	e	212	THR	5.7
1	X	88	ASP	5.7
1	Y	182	ALA	5.7
1	Y	232	PRO	5.7
1	h	237	MET	5.6
1	e	25	ASP	5.6
1	g	205	PHE	5.6
1	g	305	GLN	5.6
1	h	231	TYR	5.6
1	g	231	TYR	5.5
1	g	115	GLY	5.5
1	g	323	ILE	5.5
1	h	331	VAL	5.5
1	g	222	ILE	5.5
1	Y	43	LEU	5.5
1	b	342	MET	5.5
1	g	102	ALA	5.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	e	153	LYS	5.5
1	g	51	SER	5.5
1	e	379	LYS	5.5
1	g	21	VAL	5.5
1	g	379	LYS	5.5
1	h	162	CYS	5.5
1	U	171	GLY	5.4
1	d	450	LEU	5.4
1	h	43	LEU	5.4
1	h	158[A]	CYS	5.4
1	h	364	ARG	5.4
1	g	297	GLY	5.4
1	X	74	PHE	5.4
1	X	161	GLY	5.4
1	g	221	PRO	5.4
1	X	402	GLN	5.4
1	F	183	THR	5.4
1	X	247	PHE	5.4
1	c	58	ALA	5.4
1	h	166	THR	5.4
1	Y	74	PHE	5.4
1	I	182	ALA	5.4
1	X	87	PRO	5.4
1	X	359	PHE	5.4
1	I	371	LEU	5.4
1	h	139	GLN	5.3
1	g	154	GLN	5.3
1	h	308	ASN	5.3
1	H	100	VAL	5.3
1	e	27	TYR	5.3
1	V	331	VAL	5.3
1	e	222	ILE	5.3
1	d	98	ARG	5.3
1	g	169	HIS	5.3
1	X	386	ILE	5.3
1	H	185	CYS	5.3
1	e	359	PHE	5.3
1	g	95	ASP	5.3
1	g	316	ALA	5.3
1	h	226	ASN	5.2
1	g	314	GLN	5.2
1	d	438	ASP	5.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Y	380	ILE	5.1
1	h	106	LEU	5.1
1	Y	34	TYR	5.1
1	g	54	ASN	5.1
1	g	294	THR	5.1
1	X	452	GLU	5.1
1	e	289	SER	5.1
1	e	264	ALA	5.1
1	d	403	PHE	5.1
1	X	27	TYR	5.0
1	V	58	ALA	5.0
1	g	37	ALA	5.0
1	H	176	SER	5.0
1	i	34	TYR	5.0
1	H	148	LEU	5.0
1	h	347	GLU	5.0
1	h	255	MET	5.0
1	h	55	PRO	5.0
1	I	108	ILE	5.0
1	Y	75	ARG	5.0
1	h	468	LEU	5.0
1	X	314	GLN	5.0
1	U	59	LYS	5.0
1	V	55	PRO	4.9
1	I	172	LYS	4.9
1	X	388	THR	4.9
1	Y	238	ALA	4.9
1	U	44	ALA	4.9
1	e	43	LEU	4.9
1	g	353	THR	4.9
1	V	87	PRO	4.9
1	e	87	PRO	4.9
1	n	178	ASN	4.9
1	I	454	PHE	4.9
1	W	354	TYR	4.9
1	H	183	THR	4.9
1	e	225	CYS	4.9
1	b	205	PHE	4.8
1	I	99	LEU	4.8
1	Y	76	VAL	4.8
1	X	81	PRO	4.8
1	e	56	THR	4.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	b	363	VAL	4.8
1	g	380	ILE	4.8
1	J	61	LEU	4.8
1	d	267	LEU	4.8
1	e	239	SER	4.8
1	X	93	ASN	4.8
1	l	58	ALA	4.8
1	Z	57	ASN	4.8
1	I	20	LYS	4.8
1	c	59	LYS	4.8
1	n	180	ALA	4.8
1	d	192	ASN	4.7
1	c	90	SER	4.7
1	W	403	PHE	4.7
1	H	101	TRP	4.7
1	e	163	LYS	4.7
1	e	352	SER	4.7
1	e	293	PRO	4.7
1	d	74	PHE	4.7
1	h	203	THR	4.7
1	h	341	ASN	4.7
1	g	364	ARG	4.7
1	U	222	ILE	4.7
1	f	285	VAL	4.7
1	X	34	TYR	4.7
1	H	85	GLY	4.6
1	i	139	GLN	4.6
1	V	105	GLY	4.6
1	e	347	GLU	4.6
1	h	455	SER	4.6
1	a	105	GLY	4.6
1	V	379	LYS	4.6
1	b	45	VAL	4.6
1	g	168	GLU	4.6
1	e	215	ALA	4.6
1	g	44	ALA	4.6
1	g	152	TYR	4.6
1	f	184	ASP	4.6
1	e	20	LYS	4.6
1	X	234	TYR	4.6
1	Z	44	ALA	4.6
1	I	213	LEU	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	d	87	PRO	4.6
1	c	87	PRO	4.5
1	d	180	ALA	4.5
1	X	226	ASN	4.5
1	Y	158[A]	CYS	4.5
1	H	332	THR	4.5
1	e	193	SER	4.5
1	e	452	GLU	4.5
1	Y	453	LYS	4.5
1	W	148	LEU	4.5
1	a	275	LEU	4.5
1	g	402	GLN	4.5
1	e	89	THR	4.4
1	Y	174	VAL	4.4
1	Y	95	ASP	4.4
1	c	175	ALA	4.4
1	g	473	LEU	4.4
1	H	99	LEU	4.4
1	c	364	ARG	4.4
1	d	449	ASN	4.4
1	g	57	ASN	4.4
1	J	343	THR	4.4
1	b	74	PHE	4.4
1	h	392	THR	4.4
1	h	365	HIS	4.4
1	g	225	CYS	4.4
1	b	54	ASN	4.4
1	Y	100	VAL	4.4
1	I	106	LEU	4.4
1	Z	449	ASN	4.4
1	a	205	PHE	4.4
1	f	188	LEU	4.4
1	H	277	ILE	4.3
1	I	140	PRO	4.3
1	g	66	VAL	4.3
1	h	464	GLY	4.3
1	V	222	ILE	4.3
1	e	49	TYR	4.3
1	V	282	ASN	4.3
1	X	181	ALA	4.3
1	h	471	SER	4.3
1	Z	353	THR	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	275	LEU	4.3
1	h	228	THR	4.3
1	J	346	THR	4.3
1	g	39	SER	4.3
1	c	56	THR	4.3
1	c	141	GLY	4.3
1	i	61	LEU	4.3
1	e	294	THR	4.3
1	g	20	LYS	4.3
1	F	269	GLU	4.3
1	G	56	THR	4.3
1	I	242	TYR	4.3
1	V	74	PHE	4.3
1	h	219	ASP	4.2
1	h	470	GLN	4.2
1	g	109	GLY	4.2
1	h	340	THR	4.2
1	E	182	ALA	4.2
1	b	344	LEU	4.2
1	X	329	LEU	4.2
1	h	312	TRP	4.2
1	h	352	SER	4.2
1	F	293	PRO	4.2
1	e	197	ASP	4.2
1	X	448	VAL	4.2
1	I	380	ILE	4.2
1	e	229	CYS	4.2
1	Z	172	LYS	4.2
1	V	281	GLY	4.2
1	h	441	ASN	4.2
1	H	203	THR	4.2
1	Z	289	SER	4.2
1	Y	352	SER	4.1
1	e	96	THR	4.1
1	e	400	ASP	4.1
1	Z	59	LYS	4.1
1	e	162	CYS	4.1
1	g	183	THR	4.1
1	Y	86	PHE	4.1
1	h	80	ASP	4.1
1	h	62	LEU	4.1
1	U	182	ALA	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	g	166	THR	4.1
1	a	206	GLY	4.1
1	h	328	GLN	4.1
1	e	102	ALA	4.1
1	Y	466	LYS	4.1
1	Y	82	ASN	4.1
1	c	182	ALA	4.1
1	U	105	GLY	4.1
1	h	400	ASP	4.1
1	f	282	ASN	4.1
1	h	302	SER	4.1
1	d	378	CYS	4.1
1	F	275	LEU	4.1
1	X	76	VAL	4.1
1	g	172	LYS	4.1
1	X	358	ASN	4.1
1	h	52	ILE	4.1
1	h	99	LEU	4.1
1	e	187	PRO	4.1
1	X	305	GLN	4.0
1	H	152	TYR	4.0
1	V	44	ALA	4.0
1	e	28	VAL	4.0
1	W	120	GLY	4.0
1	Y	20	LYS	4.0
1	V	195	ILE	4.0
1	g	361	GLU	4.0
1	Y	455	SER	4.0
1	g	455	SER	4.0
1	h	358	ASN	4.0
1	I	306	LEU	4.0
1	f	186	PRO	4.0
1	e	234	TYR	4.0
1	e	319	HIS	4.0
1	U	311	TYR	4.0
1	I	398	LEU	4.0
1	g	81	PRO	4.0
1	d	179	ASN	4.0
1	b	289	SER	4.0
1	I	370	ASP	4.0
1	I	323	ILE	4.0
1	e	31	THR	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	d	401	TRP	4.0
1	g	83	LYS	4.0
1	H	445	PHE	3.9
1	V	202	ASP	3.9
1	I	378	CYS	3.9
1	X	374	VAL	3.9
1	a	45	VAL	3.9
1	V	45	VAL	3.9
1	V	473	LEU	3.9
1	g	104	VAL	3.9
1	f	52	ILE	3.9
1	d	289	SER	3.9
1	F	205	PHE	3.9
1	g	27	TYR	3.9
1	I	325	TRP	3.9
1	g	185	CYS	3.9
1	H	220	VAL	3.9
1	h	45	VAL	3.9
1	h	382	LEU	3.9
1	V	289	SER	3.9
1	X	90	SER	3.9
1	Z	171	GLY	3.9
1	V	54	ASN	3.9
1	b	57	ASN	3.9
1	g	357	GLU	3.9
1	F	132	THR	3.9
1	e	80	ASP	3.9
1	h	151	ASP	3.9
1	I	269	GLU	3.9
1	h	143	ASP	3.9
1	V	104	VAL	3.9
1	e	403	PHE	3.9
1	e	455	SER	3.9
1	g	32	SER	3.9
1	H	173	GLY	3.8
1	c	173	GLY	3.8
1	W	205	PHE	3.8
1	Y	248	PHE	3.8
1	c	86	PHE	3.8
1	Y	462	PRO	3.8
1	X	175	ALA	3.8
1	g	164	PRO	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	d	170	TRP	3.8
1	f	142	SER	3.8
1	H	363	VAL	3.8
1	h	152	TYR	3.8
1	Y	347	GLU	3.8
1	X	49	TYR	3.8
1	X	237	MET	3.8
1	d	86	PHE	3.8
1	H	151	ASP	3.8
1	h	393	MET	3.8
1	Y	397	ILE	3.8
1	g	202	ASP	3.8
1	d	226	ASN	3.8
1	h	73	VAL	3.8
1	H	115	GLY	3.8
1	I	164	PRO	3.8
1	V	35	TYR	3.8
1	e	449	ASN	3.8
1	e	292	PHE	3.8
1	Y	96	THR	3.7
1	h	371	LEU	3.7
1	h	377	LEU	3.7
1	I	205	PHE	3.7
1	W	58	ALA	3.7
1	X	318	GLY	3.7
1	H	364	ARG	3.7
1	J	342	MET	3.7
1	X	454	PHE	3.7
1	g	242	TYR	3.7
1	h	198	GLY	3.7
1	c	445	PHE	3.7
1	d	116	VAL	3.7
1	h	449	ASN	3.7
1	a	87	PRO	3.7
1	b	354	TYR	3.7
1	f	281	GLY	3.7
1	Z	58	ALA	3.7
1	h	310	PRO	3.7
1	I	190	LEU	3.7
1	e	232	PRO	3.7
1	g	318	GLY	3.7
1	h	116	VAL	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	e	97	GLN	3.7
1	h	350	LYS	3.7
1	h	388	THR	3.7
1	b	364	ARG	3.7
1	g	278	LYS	3.7
1	i	87	PRO	3.7
1	d	183	THR	3.7
1	V	275	LEU	3.7
1	g	438	ASP	3.7
1	g	333	VAL	3.7
1	X	242	TYR	3.6
1	e	189	GLU	3.6
1	H	106	LEU	3.6
1	i	329	LEU	3.6
1	S	59	LYS	3.6
1	h	74	PHE	3.6
1	H	401	TRP	3.6
1	e	353	THR	3.6
1	H	27	TYR	3.6
1	g	49	TYR	3.6
1	e	236	LYS	3.6
1	H	117	GLY	3.6
1	Y	169	HIS	3.6
1	Y	349	LYS	3.6
1	Y	390	ILE	3.6
1	f	286	ILE	3.6
1	g	60	LYS	3.6
1	h	197	ASP	3.6
1	H	190	LEU	3.6
1	h	325	TRP	3.6
1	i	81	PRO	3.6
1	I	181	ALA	3.6
1	f	353	THR	3.5
1	U	148	LEU	3.5
1	h	180	ALA	3.5
1	F	265	GLY	3.5
1	Y	388	THR	3.5
1	I	264	ALA	3.5
1	h	85	GLY	3.5
1	Y	89	THR	3.5
1	H	45	VAL	3.5
1	h	91	PHE	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	X	36	TYR	3.5
1	g	113	PRO	3.5
1	h	251	ARG	3.5
1	h	342	MET	3.5
1	e	29	SER	3.5
1	X	188	LEU	3.5
1	d	91	PHE	3.5
1	Y	446	TRP	3.5
1	N	59	LYS	3.5
1	i	56	THR	3.5
1	I	265	GLY	3.5
1	h	452	GLU	3.5
1	Y	312	TRP	3.5
1	Z	23	SER	3.5
1	e	192	ASN	3.5
1	f	172	LYS	3.5
1	Y	165	PRO	3.5
1	Z	375	PHE	3.5
1	d	159	LEU	3.5
1	h	165	PRO	3.5
1	i	35	TYR	3.5
1	W	61	LEU	3.5
1	V	269	GLU	3.5
1	V	278	LYS	3.5
1	Y	81	PRO	3.4
1	e	438	ASP	3.4
1	d	175	ALA	3.4
1	U	45	VAL	3.4
1	g	191	PHE	3.4
1	h	49	TYR	3.4
1	I	244	ASP	3.4
1	e	226	ASN	3.4
1	g	147	CYS	3.4
1	h	254	GLN	3.4
1	e	50	PHE	3.4
1	V	64	PRO	3.4
1	d	161	GLY	3.4
1	e	357	GLU	3.4
1	J	53	LYS	3.4
1	g	108	ILE	3.4
1	g	472	GLY	3.4
1	h	33	ILE	3.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	206	GLY	3.4
1	i	187	PRO	3.4
1	e	41	ARG	3.4
1	F	176	SER	3.4
1	V	364	ARG	3.4
1	X	138	ALA	3.4
1	V	79	PRO	3.4
1	J	180	ALA	3.4
1	Z	351	GLU	3.4
1	W	55	PRO	3.4
1	a	328	GLN	3.4
1	a	138	ALA	3.4
1	I	241	PRO	3.4
1	U	188	LEU	3.4
1	h	250	LEU	3.4
1	d	205	PHE	3.4
1	e	381	THR	3.4
1	F	175	ALA	3.4
1	H	44	ALA	3.4
1	X	324	CYS	3.4
1	X	159	LEU	3.4
1	X	341	ASN	3.3
1	b	61	LEU	3.3
1	g	157	LEU	3.3
1	d	448	VAL	3.3
1	V	172	LYS	3.3
1	a	398	LEU	3.3
1	V	72	ARG	3.3
1	e	402	GLN	3.3
1	h	353	THR	3.3
1	g	313	LEU	3.3
1	W	264	ALA	3.3
1	c	85	GLY	3.3
1	Y	372	GLN	3.3
1	I	327	ASN	3.3
1	U	266	LYS	3.3
1	e	95	ASP	3.3
1	h	235	LEU	3.3
1	Z	124	LEU	3.3
1	H	241	PRO	3.3
1	X	80	ASP	3.3
1	J	232	PRO	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	h	194	ILE	3.3
1	i	44	ALA	3.3
1	e	437	GLU	3.3
1	H	52	ILE	3.3
1	g	74	PHE	3.3
1	Z	402	GLN	3.3
1	Y	111	GLY	3.3
1	g	217	LYS	3.3
1	g	388	THR	3.3
1	X	50	PHE	3.3
1	e	366	VAL	3.3
1	I	255	MET	3.3
1	I	472	GLY	3.3
1	d	311	TYR	3.3
1	Y	393	MET	3.3
1	g	214	GLN	3.2
1	h	234	TYR	3.2
1	g	368	GLU	3.2
1	g	215	ALA	3.2
1	h	372	GLN	3.2
1	X	158[A]	CYS	3.2
1	e	33	ILE	3.2
1	X	346	THR	3.2
1	n	58	ALA	3.2
1	U	120	GLY	3.2
1	X	232	PRO	3.2
1	e	346	THR	3.2
1	d	45	VAL	3.2
1	U	172	LYS	3.2
1	a	153	LYS	3.2
1	h	51	SER	3.2
1	H	191	PHE	3.2
1	F	288	SER	3.2
1	I	399	GLU	3.2
1	I	139	GLN	3.2
1	V	329	LEU	3.2
1	Y	195	ILE	3.2
1	d	188	LEU	3.2
1	g	148	LEU	3.2
1	j	55	PRO	3.2
1	e	169	HIS	3.2
1	V	380	ILE	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	b	294	THR	3.2
1	h	247	PHE	3.2
1	Y	265	GLY	3.2
1	h	167	GLY	3.2
1	g	352	SER	3.2
1	Y	389	TYR	3.2
1	c	101	TRP	3.2
1	c	174	VAL	3.2
1	e	51	SER	3.2
1	f	205	PHE	3.2
1	h	64	PRO	3.2
1	H	357	GLU	3.2
1	U	43	LEU	3.2
1	a	288	SER	3.2
1	X	222	ILE	3.2
1	g	56	THR	3.2
1	g	329	LEU	3.2
1	F	264	ALA	3.2
1	X	192	ASN	3.2
1	H	381	THR	3.2
1	V	93	ASN	3.1
1	V	188	LEU	3.1
1	h	221	PRO	3.1
1	e	53	LYS	3.1
1	a	289	SER	3.1
1	g	40	SER	3.1
1	b	85	GLY	3.1
1	F	131	GLU	3.1
1	J	55	PRO	3.1
1	h	87	PRO	3.1
1	i	375	PHE	3.1
1	X	378	CYS	3.1
1	H	265	GLY	3.1
1	e	401	TRP	3.1
1	Z	363	VAL	3.1
1	Y	400	ASP	3.1
1	X	365	HIS	3.1
1	I	331	VAL	3.1
1	a	72	ARG	3.1
1	a	114	LEU	3.1
1	e	52	ILE	3.1
1	e	55	PRO	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	342	MET	3.1
1	V	98	ARG	3.1
1	V	393	MET	3.1
1	i	57	ASN	3.1
1	e	23	SER	3.1
1	c	46	GLY	3.1
1	g	456	ALA	3.1
1	g	116	VAL	3.1
1	i	74	PHE	3.1
1	I	452	GLU	3.1
1	J	182	ALA	3.1
1	I	158[A]	CYS	3.1
1	d	153	LYS	3.1
1	J	74	PHE	3.1
1	W	445	PHE	3.1
1	V	95	ASP	3.1
1	g	25	ASP	3.1
1	c	74	PHE	3.1
1	Y	280	SER	3.1
1	X	195	ILE	3.1
1	d	81	PRO	3.1
1	G	289	SER	3.1
1	I	149	SER	3.1
1	e	380	ILE	3.1
1	W	46	GLY	3.1
1	I	456	ALA	3.0
1	H	219	ASP	3.0
1	e	451	LYS	3.0
1	I	101	TRP	3.0
1	V	402	GLN	3.0
1	Z	148	LEU	3.0
1	c	165	PRO	3.0
1	c	401	TRP	3.0
1	g	228	THR	3.0
1	h	138	ALA	3.0
1	X	367	GLU	3.0
1	a	269	GLU	3.0
1	h	244	ASP	3.0
1	h	274	ASP	3.0
1	g	118	VAL	3.0
1	h	296	SER	3.0
1	c	139	GLN	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	b	325	TRP	3.0
1	a	38	GLY	3.0
1	i	347	GLU	3.0
1	e	214	GLN	3.0
1	h	191	PHE	3.0
1	e	121	HIS	3.0
1	X	41	ARG	3.0
1	e	60	LYS	3.0
1	W	45	VAL	3.0
1	i	348	VAL	3.0
1	I	393	MET	3.0
1	e	457	ASP	3.0
1	f	127	PHE	3.0
1	J	356	ASN	3.0
1	d	82	ASN	3.0
1	e	216	ASN	3.0
1	g	355	LYS	3.0
1	a	448	VAL	3.0
1	J	56	THR	2.9
1	I	403	PHE	2.9
1	d	207	CYS	2.9
1	e	368	GLU	2.9
1	g	237	MET	2.9
1	Y	91	PHE	2.9
1	Y	44	ALA	2.9
1	e	120	GLY	2.9
1	X	379	LYS	2.9
1	d	458	LEU	2.9
1	K	182	ALA	2.9
1	U	147	CYS	2.9
1	H	91	PHE	2.9
1	I	298	SER	2.9
1	G	139	GLN	2.9
1	V	160	ILE	2.9
1	n	179	ASN	2.9
1	Z	448	VAL	2.9
1	h	172	LYS	2.9
1	a	387	MET	2.9
1	d	103	CYS	2.9
1	I	369	TYR	2.9
1	c	103	CYS	2.9
1	h	103	CYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	182	ALA	2.9
1	g	370	ASP	2.9
1	Y	363	VAL	2.9
1	g	139	GLN	2.9
1	Y	207	CYS	2.9
1	H	275	LEU	2.9
1	d	44	ALA	2.9
1	e	244	ASP	2.9
1	i	364	ARG	2.9
1	b	403	PHE	2.9
1	h	112	GLN	2.9
1	V	109	GLY	2.9
1	a	109	GLY	2.9
1	X	357	GLU	2.9
1	e	448	VAL	2.9
1	Y	25	ASP	2.9
1	f	187	PRO	2.9
1	F	317	GLN	2.9
1	h	337	THR	2.8
1	i	105	GLY	2.8
1	H	142	SER	2.8
1	F	206	GLY	2.8
1	Z	342	MET	2.8
1	H	120	GLY	2.8
1	I	254	GLN	2.8
1	i	356	ASN	2.8
1	n	182	ALA	2.8
1	Y	364	ARG	2.8
1	Z	364	ARG	2.8
1	Z	266	LYS	2.8
1	X	457	ASP	2.8
1	I	55	PRO	2.8
1	e	444	THR	2.8
1	U	71	TYR	2.8
1	d	34	TYR	2.8
1	d	172	LYS	2.8
1	g	300	VAL	2.8
1	V	291	PHE	2.8
1	h	351	GLU	2.8
1	Y	293	PRO	2.8
1	V	268	GLY	2.8
1	X	366	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Z	220	VAL	2.8
1	h	265	GLY	2.8
1	Z	121	HIS	2.8
1	h	305	GLN	2.8
1	I	195	ILE	2.8
1	V	261	PHE	2.8
1	d	393	MET	2.8
1	U	282	ASN	2.8
1	Y	186	PRO	2.8
1	a	152	TYR	2.8
1	H	108	ILE	2.8
1	J	364	ARG	2.8
1	e	90	SER	2.8
1	g	90	SER	2.8
1	I	45	VAL	2.8
1	h	118	VAL	2.8
1	I	171	GLY	2.8
1	d	93	ASN	2.8
1	d	190	LEU	2.8
1	g	371	LEU	2.8
1	h	333	VAL	2.8
1	Z	188	LEU	2.8
1	F	65	LYS	2.8
1	U	122	PRO	2.8
1	d	88	ASP	2.8
1	c	45	VAL	2.8
1	e	460	GLN	2.8
1	i	343	THR	2.8
1	Z	288	SER	2.8
1	U	190	LEU	2.8
1	J	41	ARG	2.8
1	X	97	GLN	2.8
1	X	32	SER	2.8
1	c	190	LEU	2.8
1	g	117	GLY	2.8
1	h	463	LEU	2.8
1	F	201	VAL	2.8
1	V	449	ASN	2.8
1	h	173	GLY	2.8
1	i	112	GLN	2.7
1	A	182	ALA	2.7
1	G	288	SER	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	109	GLY	2.7
1	I	148	LEU	2.7
1	e	375	PHE	2.7
1	g	359	PHE	2.7
1	J	331	VAL	2.7
1	Z	222	ILE	2.7
1	a	363	VAL	2.7
1	g	174	VAL	2.7
1	I	361	GLU	2.7
1	a	329	LEU	2.7
1	H	50	PHE	2.7
1	e	312	TRP	2.7
1	g	387	MET	2.7
1	h	56	THR	2.7
1	Z	192	ASN	2.7
1	U	402	GLN	2.7
1	I	79	PRO	2.7
1	U	186	PRO	2.7
1	V	136	TYR	2.7
1	g	53	LYS	2.7
1	W	342	MET	2.7
1	X	385	GLU	2.7
1	X	394	ASP	2.7
1	F	363	VAL	2.7
1	a	76	VAL	2.7
1	a	375	PHE	2.7
1	e	199	ASP	2.7
1	F	290	ALA	2.7
1	X	94	PRO	2.7
1	e	298	SER	2.7
1	h	105	GLY	2.7
1	i	327	ASN	2.7
1	G	172	LYS	2.7
1	Y	159	LEU	2.7
1	J	81	PRO	2.7
1	X	51	SER	2.7
1	X	330	PHE	2.7
1	b	60	LYS	2.7
1	X	316	ALA	2.7
1	Z	46	GLY	2.7
1	e	307	PHE	2.7
1	g	346	THR	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	X	63	VAL	2.7
1	a	331	VAL	2.7
1	i	104	VAL	2.7
1	G	204	GLY	2.7
1	J	347	GLU	2.7
1	a	44	ALA	2.7
1	i	180	ALA	2.7
1	Q	59	LYS	2.7
1	V	214	GLN	2.7
1	X	268	GLY	2.7
1	I	278	LYS	2.7
1	F	213	LEU	2.7
1	W	344	LEU	2.7
1	Y	454	PHE	2.7
1	d	371	LEU	2.7
1	h	122	PRO	2.7
1	X	370	ASP	2.7
1	U	173	GLY	2.7
1	Y	60	LYS	2.7
1	W	98	ARG	2.6
1	a	35	TYR	2.6
1	h	472	GLY	2.6
1	Y	57	ASN	2.6
1	e	47	ASN	2.6
1	F	225	CYS	2.6
1	Y	203	THR	2.6
1	d	334	VAL	2.6
1	U	112	GLN	2.6
1	I	377	LEU	2.6
1	V	378	CYS	2.6
1	d	92	TYR	2.6
1	e	447	GLU	2.6
1	Y	360	LYS	2.6
1	a	241	PRO	2.6
1	b	103	CYS	2.6
1	d	60	LYS	2.6
1	X	52	ILE	2.6
1	X	380	ILE	2.6
1	X	449	ASN	2.6
1	Y	98	ARG	2.6
1	Y	175	ALA	2.6
1	a	115	GLY	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	e	318	GLY	2.6
1	U	351	GLU	2.6
1	e	273	ASP	2.6
1	I	249	PHE	2.6
1	b	27	TYR	2.6
1	d	132	THR	2.6
1	W	175	ALA	2.6
1	c	167	GLY	2.6
1	h	298	SER	2.6
1	h	447	GLU	2.6
1	g	384	ALA	2.6
1	J	139	GLN	2.6
1	Q	139	GLN	2.6
1	X	466	LYS	2.6
1	h	339	SER	2.6
1	e	190	LEU	2.6
1	Y	444	THR	2.6
1	i	448	VAL	2.6
1	F	55	PRO	2.6
1	V	346	THR	2.6
1	X	440	LEU	2.6
1	V	46	GLY	2.6
1	a	100	VAL	2.6
1	d	90	SER	2.6
1	e	166	THR	2.6
1	h	81	PRO	2.6
1	H	188	LEU	2.6
1	W	131	GLU	2.6
1	h	86	PHE	2.6
1	H	342	MET	2.6
1	I	289	SER	2.6
1	W	153	LYS	2.6
1	U	386	ILE	2.6
1	d	164	PRO	2.6
1	e	64	PRO	2.6
1	V	170	TRP	2.6
1	d	276	TYR	2.6
1	e	200	MET	2.6
1	h	208	MET	2.6
1	k	139	GLN	2.6
1	X	333	VAL	2.6
1	T	179	ASN	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	43	LEU	2.6
1	h	124	LEU	2.6
1	U	170	TRP	2.6
1	h	238	ALA	2.6
1	I	373	PHE	2.6
1	X	191	PHE	2.6
1	I	87	PRO	2.5
1	J	179	ASN	2.5
1	V	468	LEU	2.5
1	a	132	THR	2.5
1	h	346	THR	2.5
1	b	53	LYS	2.5
1	a	255	MET	2.5
1	Y	41	ARG	2.5
1	X	21	VAL	2.5
1	e	331	VAL	2.5
1	d	178	ASN	2.5
1	m	140	PRO	2.5
1	V	273	ASP	2.5
1	f	265	GLY	2.5
1	X	340	THR	2.5
1	a	450	LEU	2.5
1	X	298	SER	2.5
1	h	174	VAL	2.5
1	V	325	TRP	2.5
1	c	243	GLY	2.5
1	g	114	LEU	2.5
1	i	267	LEU	2.5
1	V	53	LYS	2.5
1	h	318	GLY	2.5
1	G	188	LEU	2.5
1	b	195	ILE	2.5
1	e	358	ASN	2.5
1	d	117	GLY	2.5
1	I	382	LEU	2.5
1	d	220	VAL	2.5
1	h	76	VAL	2.5
1	g	96	THR	2.5
1	F	268	GLY	2.5
1	X	101	TRP	2.5
1	X	450	LEU	2.5
1	X	356	ASN	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	53	LYS	2.5
1	Y	173	GLY	2.5
1	U	27	TYR	2.5
1	X	229	CYS	2.5
1	a	27	TYR	2.5
1	F	403	PHE	2.5
1	b	153	LYS	2.5
1	e	247	PHE	2.5
1	e	387	MET	2.5
1	g	206	GLY	2.5
1	V	52	ILE	2.5
1	g	471	SER	2.5
1	V	27	TYR	2.5
1	a	52	ILE	2.5
1	a	343	THR	2.5
1	e	155	THR	2.5
1	n	382	LEU	2.5
1	a	137	PRO	2.5
1	E	181	ALA	2.5
1	e	206	GLY	2.5
1	b	277	ILE	2.5
1	F	220	VAL	2.5
1	a	238	ALA	2.5
1	H	379	LYS	2.5
1	c	176	SER	2.5
1	e	295	PRO	2.5
1	F	44	ALA	2.5
1	I	326	GLY	2.5
1	g	150	MET	2.5
1	I	153	LYS	2.5
1	h	467	PHE	2.5
1	H	361	GLU	2.4
1	I	354	TYR	2.4
1	g	82	ASN	2.4
1	e	171	GLY	2.4
1	K	403	PHE	2.4
1	H	346	THR	2.4
1	U	114	LEU	2.4
1	a	237	MET	2.4
1	c	380	ILE	2.4
1	b	148	LEU	2.4
1	g	36	TYR	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	68	GLY	2.4
1	a	366	VAL	2.4
1	d	376	GLN	2.4
1	h	288	SER	2.4
1	a	325	TRP	2.4
1	F	126	LYS	2.4
1	I	324	CYS	2.4
1	V	76	VAL	2.4
1	G	52	ILE	2.4
1	P	182	ALA	2.4
1	g	274	ASP	2.4
1	c	358	ASN	2.4
1	Z	382	LEU	2.4
1	e	364	ARG	2.4
1	V	38	GLY	2.4
1	U	35	TYR	2.4
1	b	271	VAL	2.4
1	F	138	ALA	2.4
1	H	264	ALA	2.4
1	W	86	PHE	2.4
1	f	215	ALA	2.4
1	c	383	THR	2.4
1	e	36	TYR	2.4
1	F	120	GLY	2.4
1	H	307	PHE	2.4
1	V	138	ALA	2.4
1	b	264	ALA	2.4
1	d	238	ALA	2.4
1	P	389	TYR	2.4
1	g	273	ASP	2.4
1	d	195	ILE	2.4
1	V	292	PHE	2.4
1	e	297	GLY	2.4
1	d	277	ILE	2.4
1	X	54	ASN	2.4
1	Z	281	GLY	2.4
1	Z	264	ALA	2.4
1	H	114	LEU	2.4
1	X	382	LEU	2.4
1	e	158[A]	CYS	2.4
1	U	51	SER	2.4
1	I	215	ALA	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	371	LEU	2.4
1	V	100	VAL	2.4
1	Z	374	VAL	2.4
1	g	107	GLU	2.4
1	H	61	LEU	2.4
1	c	132	THR	2.4
1	h	44	ALA	2.4
1	H	86	PHE	2.4
1	W	195	ILE	2.4
1	X	269	GLU	2.4
1	e	330	PHE	2.4
1	e	397	ILE	2.4
1	V	43	LEU	2.4
1	H	48	PRO	2.4
1	g	454	PHE	2.4
1	H	204	GLY	2.4
1	I	208	MET	2.4
1	V	464	GLY	2.4
1	W	289	SER	2.4
1	X	106	LEU	2.4
1	c	166	THR	2.4
1	H	367	GLU	2.4
1	J	349	LYS	2.4
1	Y	33	ILE	2.4
1	a	361	GLU	2.4
1	d	55	PRO	2.4
1	g	470	GLN	2.4
1	h	299	ILE	2.4
1	W	201	VAL	2.4
1	d	215	ALA	2.4
1	I	152	TYR	2.4
1	V	394	ASP	2.4
1	h	184	ASP	2.4
1	g	299	ILE	2.3
1	h	301	THR	2.4
1	n	59	LYS	2.4
1	U	111	GLY	2.3
1	E	180	ALA	2.3
1	i	159	LEU	2.3
1	L	59	LYS	2.3
1	V	403	PHE	2.3
1	c	352	SER	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	g	459	ASP	2.3
1	g	453	LYS	2.3
1	h	229	CYS	2.3
1	d	235	LEU	2.3
1	d	257	VAL	2.3
1	a	259	HIS	2.3
1	d	466	LYS	2.3
1	e	324	CYS	2.3
1	I	352	SER	2.3
1	a	473	LEU	2.3
1	m	106	LEU	2.3
1	X	56	THR	2.3
1	Y	55	PRO	2.3
1	E	403	PHE	2.3
1	f	120	GLY	2.3
1	Y	244	ASP	2.3
1	h	453	LYS	2.3
1	i	98	ARG	2.3
1	a	43	LEU	2.3
1	e	367	GLU	2.3
1	Y	379	LYS	2.3
1	V	343	THR	2.3
1	F	69	LEU	2.3
1	X	343	THR	2.3
1	a	380	ILE	2.3
1	c	186	PRO	2.3
1	H	371	LEU	2.3
1	U	366	VAL	2.3
1	i	188	LEU	2.3
1	h	169	HIS	2.3
1	d	102	ALA	2.3
1	f	284	ALA	2.3
1	C	460	GLN	2.3
1	X	272	PRO	2.3
1	X	372	GLN	2.3
1	a	222	ILE	2.3
1	d	214	GLN	2.3
1	I	366	VAL	2.3
1	U	329	LEU	2.3
1	Y	398	LEU	2.3
1	d	266	LYS	2.3
1	i	374	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	e	30	ARG	2.3
1	g	101	TRP	2.3
1	g	341	ASN	2.3
1	X	35	TYR	2.3
1	j	448	VAL	2.3
1	h	204	GLY	2.3
1	c	195	ILE	2.3
1	K	382	LEU	2.3
1	U	358	ASN	2.3
1	G	205	PHE	2.3
1	H	166	THR	2.3
1	H	208	MET	2.3
1	W	85	GLY	2.3
1	Y	337	THR	2.3
1	d	206	GLY	2.3
1	F	341	ASN	2.3
1	d	174	VAL	2.3
1	g	298	SER	2.3
1	g	120	GLY	2.3
1	H	382	LEU	2.3
1	H	291	PHE	2.3
1	V	241	PRO	2.3
1	g	308	ASN	2.3
1	e	342	MET	2.3
1	H	153	LYS	2.3
1	g	223	ASP	2.3
1	e	118	VAL	2.3
1	h	220	VAL	2.3
1	d	384	ALA	2.3
1	g	93	ASN	2.3
1	F	129	ASP	2.3
1	g	89	THR	2.3
1	Y	289	SER	2.2
1	F	401	TRP	2.2
1	F	203	THR	2.2
1	F	149	SER	2.2
1	V	207	CYS	2.2
1	d	186	PRO	2.2
1	I	188	LEU	2.2
1	e	314	GLN	2.2
1	Z	299	ILE	2.2
1	W	236	LYS	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	447	GLU	2.2
1	V	277	ILE	2.2
1	I	395	SER	2.2
1	W	364	ARG	2.2
1	g	263	ARG	2.2
1	g	360	LYS	2.2
1	h	107	GLU	2.2
1	I	464	GLY	2.2
1	J	277	ILE	2.2
1	U	68	GLY	2.2
1	d	402	GLN	2.2
1	h	181	ALA	2.2
1	F	153	LYS	2.2
1	H	266	LYS	2.2
1	I	248	PHE	2.2
1	a	91	PHE	2.2
1	g	330	PHE	2.2
1	V	36	TYR	2.2
1	c	447	GLU	2.2
1	G	220	VAL	2.2
1	I	62	LEU	2.2
1	Y	68	GLY	2.2
1	e	473	LEU	2.2
1	G	126	LYS	2.2
1	H	53	LYS	2.2
1	H	119	SER	2.2
1	Y	239	SER	2.2
1	V	159	LEU	2.2
1	d	105	GLY	2.2
1	d	367	GLU	2.2
1	d	379	LYS	2.2
1	G	55	PRO	2.2
1	e	327	ASN	2.2
1	g	320	ASN	2.2
1	V	389	TYR	2.2
1	X	444	THR	2.2
1	Y	375	PHE	2.2
1	h	460	GLN	2.2
1	F	343	THR	2.2
1	e	392	THR	2.2
1	h	21	VAL	2.2
1	U	210	PHE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	g	112	GLN	2.2
1	G	269	GLU	2.2
1	H	233	ASP	2.2
1	Z	450	LEU	2.2
1	c	386	ILE	2.2
1	g	153	LYS	2.2
1	Z	232	PRO	2.2
1	h	275	LEU	2.2
1	H	150	MET	2.2
1	J	302	SER	2.2
1	d	264	ALA	2.2
1	f	139	GLN	2.2
1	d	453	LYS	2.2
1	h	69	LEU	2.2
1	I	330	PHE	2.2
1	I	282	ASN	2.2
1	c	125	ASN	2.2
1	h	223	ASP	2.2
1	e	119	SER	2.2
1	g	218	SER	2.2
1	R	35	TYR	2.2
1	g	61	LEU	2.2
1	i	450	LEU	2.2
1	c	403	PHE	2.2
1	U	387	MET	2.2
1	F	244	ASP	2.2
1	c	242	TYR	2.2
1	d	35	TYR	2.2
1	i	160	ILE	2.2
1	V	187	PRO	2.1
1	c	120	GLY	2.1
1	I	59	LYS	2.1
1	V	324	CYS	2.1
1	g	77	ARG	2.1
1	Y	194	ILE	2.1
1	J	72	ARG	2.1
1	g	126	LYS	2.1
1	S	179	ASN	2.1
1	H	351	GLU	2.1
1	Y	324	CYS	2.1
1	Z	277	ILE	2.1
1	d	39	SER	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	X	317	GLN	2.1
1	e	198	GLY	2.1
1	h	387	MET	2.1
1	F	174	VAL	2.1
1	V	61	LEU	2.1
1	b	275	LEU	2.1
1	H	68	GLY	2.1
1	I	245	SER	2.1
1	a	203	THR	2.1
1	a	353	THR	2.1
1	c	373	PHE	2.1
1	g	400	ASP	2.1
1	H	207	CYS	2.1
1	G	366	VAL	2.1
1	I	86	PHE	2.1
1	b	362	TYR	2.1
1	Y	212	THR	2.1
1	V	285	VAL	2.1
1	Y	58	ALA	2.1
1	Y	106	LEU	2.1
1	b	200	MET	2.1
1	d	165	PRO	2.1
1	U	152	TYR	2.1
1	K	380	ILE	2.1
1	i	403	PHE	2.1
1	U	169	HIS	2.1
1	F	200	MET	2.1
1	I	192	ASN	2.1
1	U	106	LEU	2.1
1	c	159	LEU	2.1
1	h	114	LEU	2.1
1	h	185	CYS	2.1
1	I	439	PRO	2.1
1	b	165	PRO	2.1
1	a	172	LYS	2.1
1	f	141	GLY	2.1
1	G	290	ALA	2.1
1	X	377	LEU	2.1
1	a	188	LEU	2.1
1	c	246	LEU	2.1
1	g	175	ALA	2.1
1	g	250	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	i	182	ALA	2.1
1	J	36	TYR	2.1
1	g	47	ASN	2.1
1	e	160	ILE	2.1
1	h	307	PHE	2.1
1	h	115	GLY	2.1
1	i	114	LEU	2.1
1	H	149	SER	2.1
1	i	54	ASN	2.1
1	i	380	ILE	2.1
1	h	271	VAL	2.1
1	F	23	SER	2.1
1	X	110	ARG	2.1
1	J	468	LEU	2.1
1	g	382	LEU	2.1
1	d	360	LYS	2.1
1	U	364	ARG	2.1
1	Y	132	THR	2.1
1	a	103	CYS	2.1
1	f	212	THR	2.1
1	f	241	PRO	2.1
1	V	450	LEU	2.1
1	i	76	VAL	2.1
1	I	387	MET	2.1
1	Y	463	LEU	2.1
1	Z	120	GLY	2.1
1	j	183	THR	2.1
1	H	57	ASN	2.1
1	a	330	PHE	2.1
1	c	181	ALA	2.1
1	d	84	PHE	2.1
1	C	176	SER	2.1
1	a	351	GLU	2.1
1	g	149	SER	2.1
1	O	180	ALA	2.1
1	V	290	ALA	2.1
1	V	362	TYR	2.1
1	Y	311	TYR	2.1
1	b	226	ASN	2.1
1	H	39	SER	2.1
1	G	222	ILE	2.1
1	W	185	CYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	V	49	TYR	2.1
1	d	397	ILE	2.1
1	W	57	ASN	2.1
1	J	105	GLY	2.1
1	i	278	LYS	2.0
1	W	369	TYR	2.0
1	I	473	LEU	2.0
1	U	313	LEU	2.0
1	Y	366	VAL	2.0
1	Y	171	GLY	2.0
1	c	205	PHE	2.0
1	U	175	ALA	2.0
1	Y	237	MET	2.0
1	e	439	PRO	2.0
1	J	345	CYS	2.0
1	Y	343	THR	2.0
1	Y	459	ASP	2.0
1	c	343	THR	2.0
1	e	103	CYS	2.0
1	Y	472	GLY	2.0
1	a	74	PHE	2.0
1	c	171	GLY	2.0
1	e	322	GLY	2.0
1	d	386	ILE	2.0
1	g	35	TYR	2.0
1	F	199	ASP	2.0
1	V	148	LEU	2.0
1	g	366	VAL	2.0
1	g	444	THR	2.0
1	Y	243	GLY	2.0
1	g	198	GLY	2.0
1	F	350	LYS	2.0
1	H	88	ASP	2.0
1	W	103	CYS	2.0
1	h	37	ALA	2.0
1	W	126	LYS	2.0
1	W	169	HIS	2.0
1	h	20	LYS	2.0
1	h	454	PHE	2.0
1	G	183	THR	2.0
1	h	385	GLU	2.0
1	m	44	ALA	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	267	LEU	2.0
1	Z	311	TYR	2.0
1	Y	84	PHE	2.0
1	c	350	LYS	2.0
1	d	106	LEU	2.0
1	Y	90	SER	2.0
1	I	117	GLY	2.0
1	g	447	GLU	2.0
1	n	357	GLU	2.0
1	a	160	ILE	2.0
1	U	213	LEU	2.0
1	X	312	TRP	2.0
1	d	76	VAL	2.0
1	h	266	LYS	2.0
1	U	293	PRO	2.0
1	Z	74	PHE	2.0
1	a	292	PHE	2.0
1	g	165	PRO	2.0

## 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 monosaccharides 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.