



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 11:12 AM UTC

PDB ID : 6IGC / pdb_00006igc
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

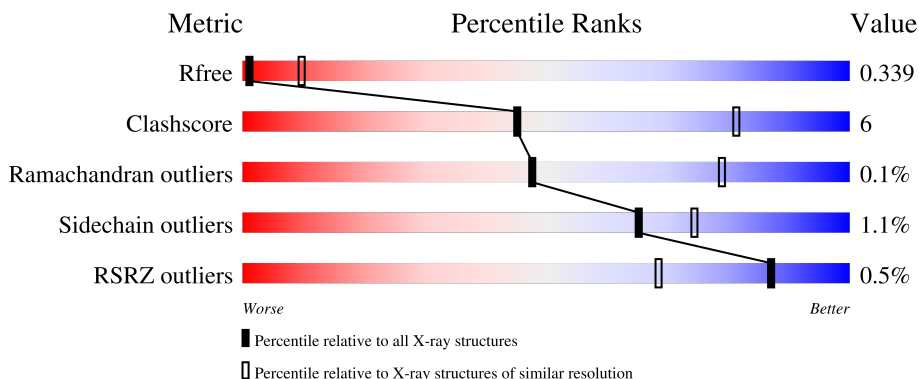
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 68% 11% 20%
1	B	524	 68% 11% 21%
1	C	524	 72% 8% 21%
1	D	524	 68% 11% 21%
1	E	524	 68% 11% 21%

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Mol	Chain	Length	Quality of chain
1	F	524	66% 13% 21%
1	G	524	69% 10% 21%
1	H	524	69% 10% 21%
1	I	524	68% 12% 20%
1	J	524	68% 12% 20%
1	K	524	66% 13% 21%
1	L	524	69% 10% 21%
1	M	524	67% 12% 21%
1	N	524	66% 12% 21%
1	O	524	68% 12% 20%
1	P	524	70% 9% 21%
1	Q	524	70% 9% 21%
1	R	524	70% 9% 21%
1	S	524	69% 11% 20%
1	T	524	69% 11% 20%
1	U	524	65% 13% 21%
1	V	524	68% 11% 21%
1	W	524	56% 22% 21%
1	X	524	56% 23% 20%
1	Y	524	67% 13% 20%
1	Z	524	67% 11% 21%
1	a	524	68% 11% 21%
1	b	524	69% 10% 21%
1	c	524	68% 12% 20%
1	d	524	68% 11% 20%

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Mol	Chain	Length	Quality of chain
1	e	524	<p>% 59% 19% 21%</p>
1	f	524	<p>62% 17% 21%</p>
1	g	524	<p>% 67% 12% 21%</p>
1	h	524	<p>68% 12% 20%</p>
1	i	524	<p>% 67% 13% 20%</p>
1	j	524	<p>% 69% 10% 21%</p>
1	k	524	<p>71% 8% 21%</p>
1	l	524	<p>71% 8% 21%</p>
1	m	524	<p>70% 9% 20%</p>
1	n	524	<p>69% 10% 20%</p>

2 Entry composition [i](#)

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

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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			

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

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

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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

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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

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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

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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

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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

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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

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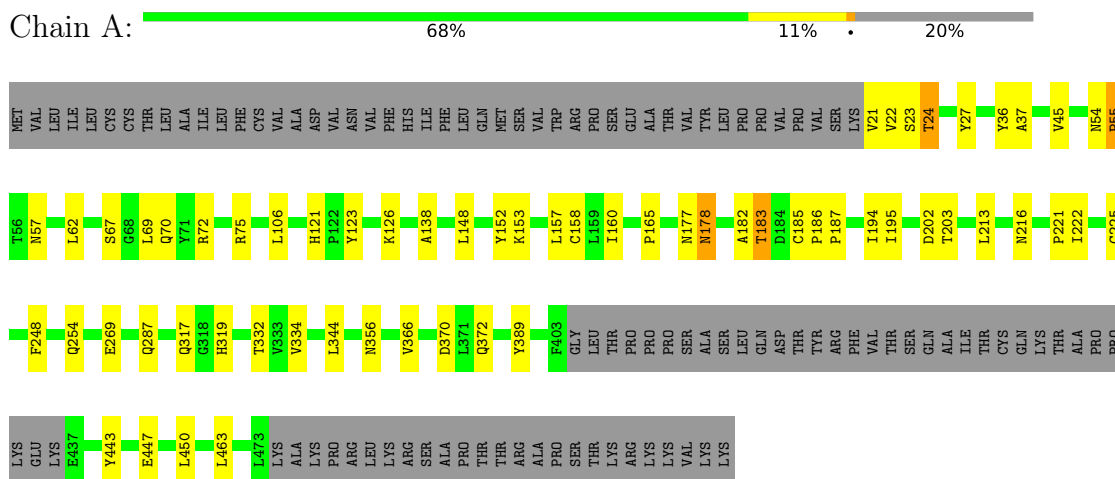
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Chain	Residue	Modelled	Actual	Comment	Reference
j	176	SER	CYS	engineered mutation	UNP P26535
j	349	LYS	THR	engineered mutation	UNP P26535
j	352	SER	GLY	engineered mutation	UNP P26535
j	357	GLU	ASP	engineered mutation	UNP P26535
k	54	ASN	SER	engineered 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

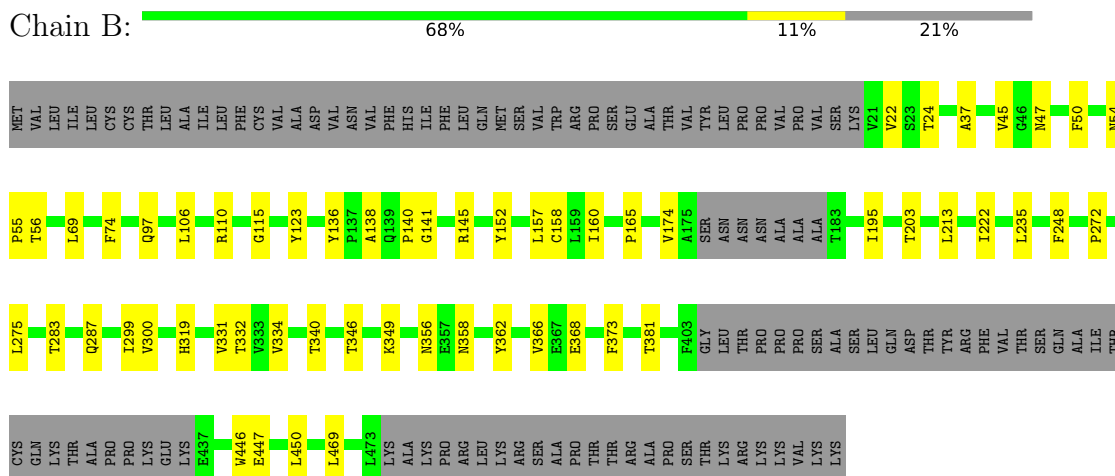
3 Residue-property plots [i](#)

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

- Molecule 1: Major capsid protein L1

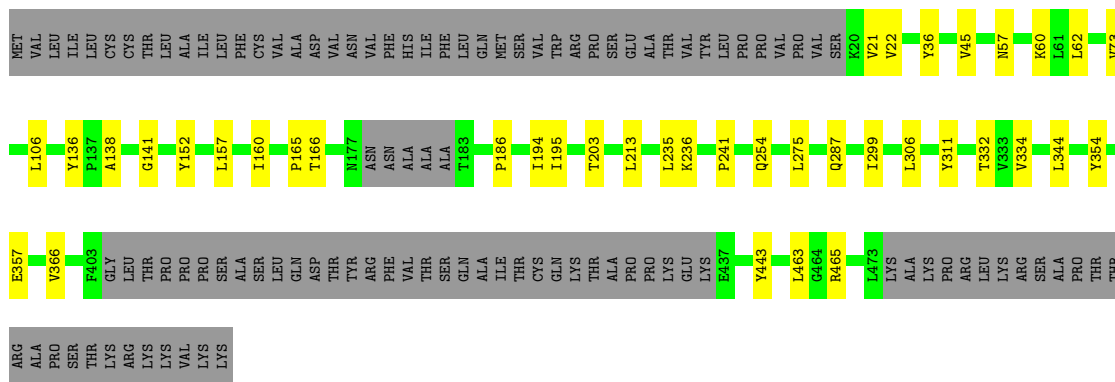


- Molecule 1: Major capsid protein L1

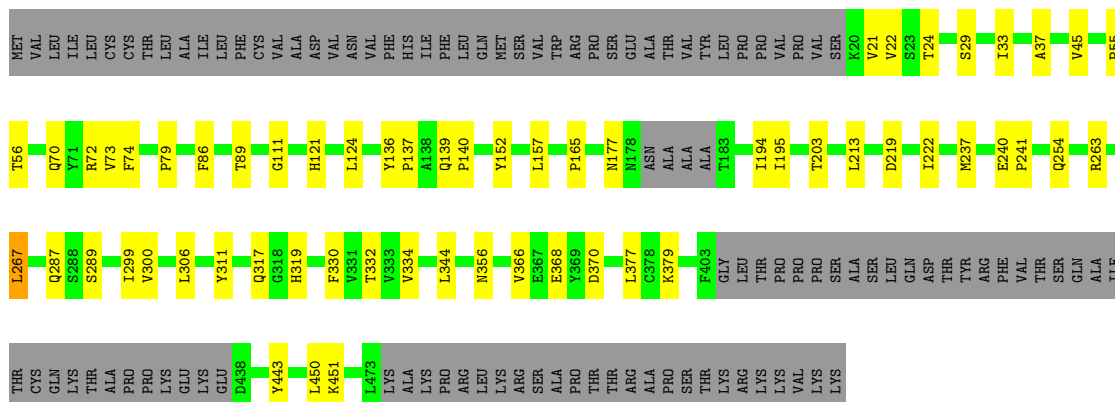


- Molecule 1: Major capsid protein L1

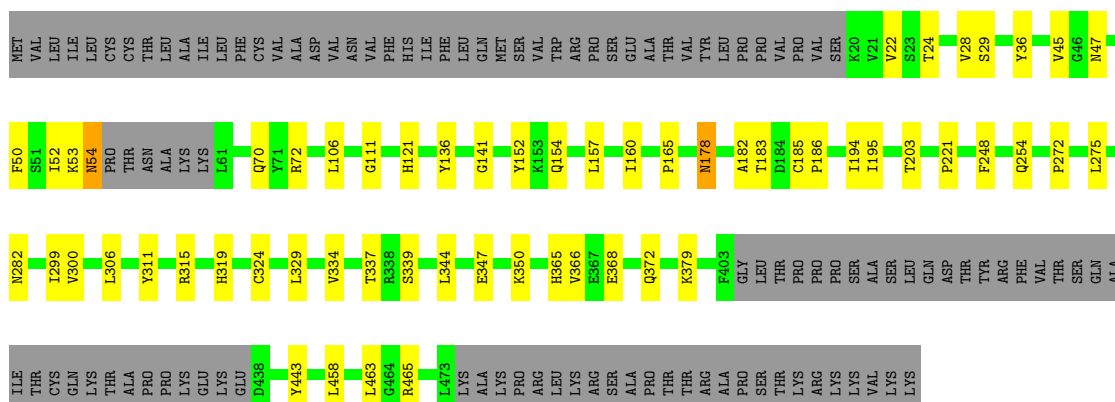




• Molecule 1: Major capsid protein L1

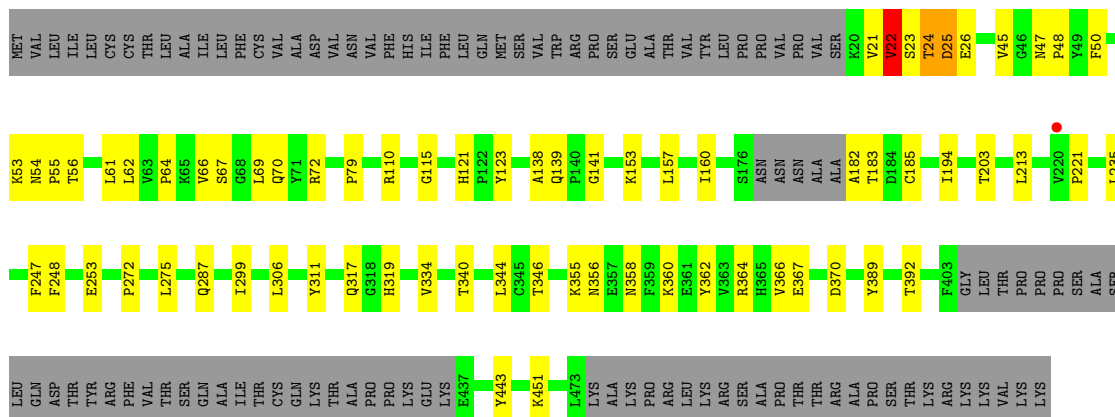


• Molecule 1: Major capsid protein L1

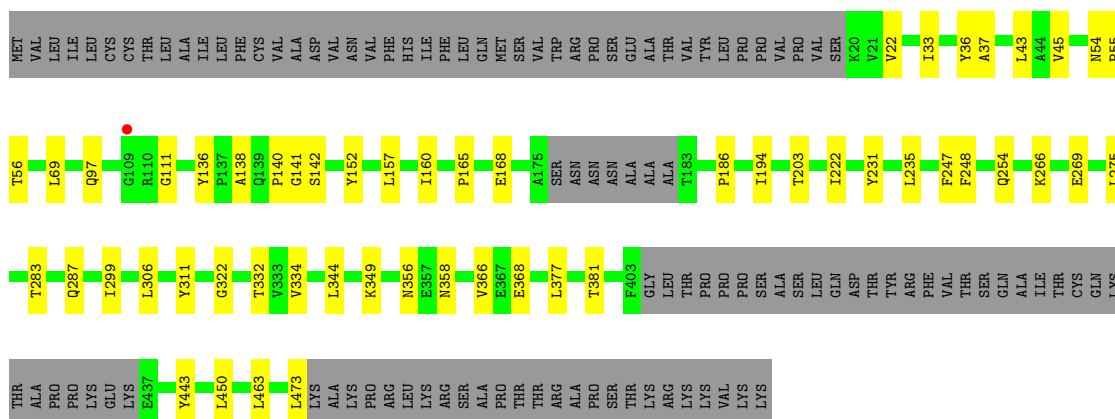


• Molecule 1: Major capsid protein L1

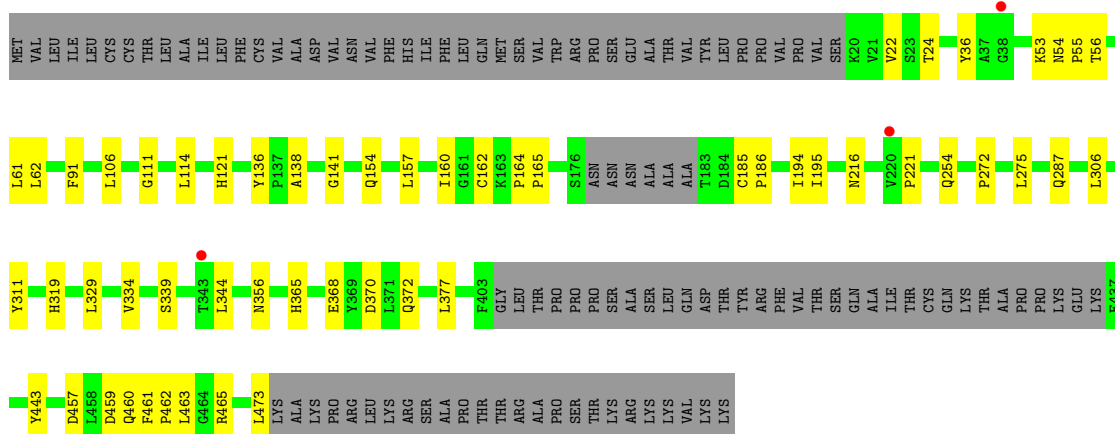




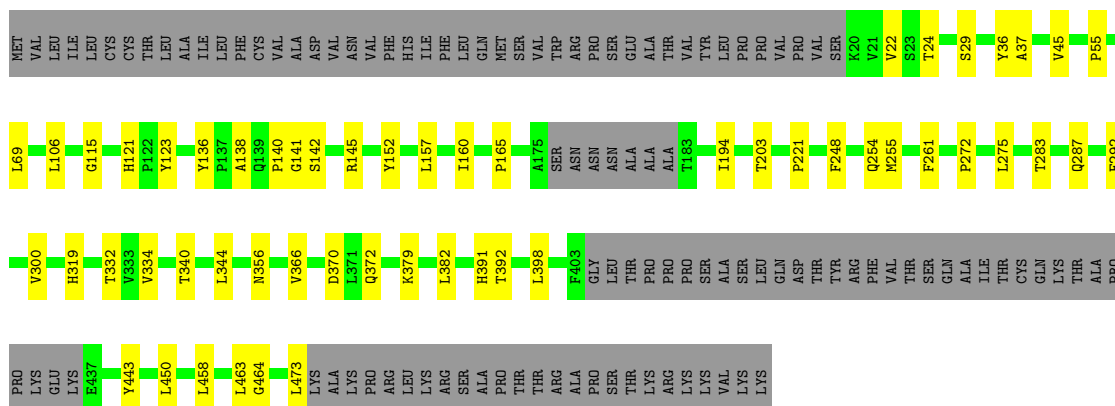
● Molecule 1: Major capsid protein L1



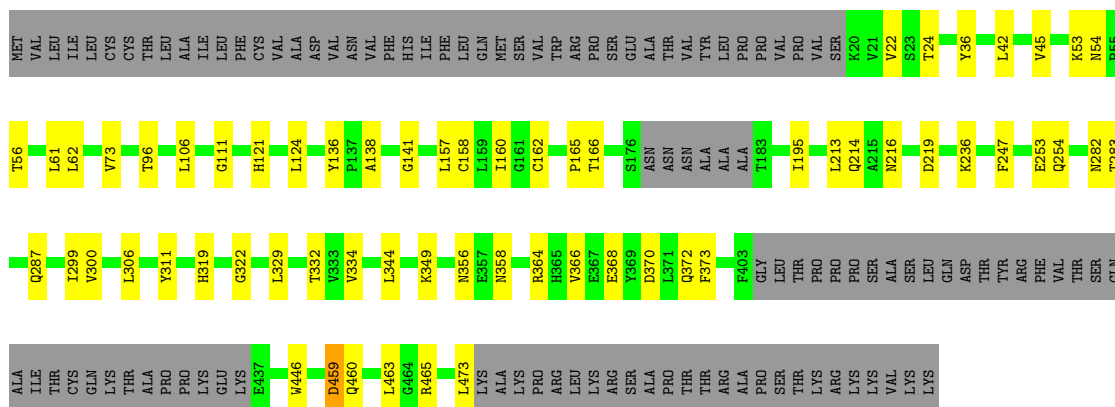
● Molecule 1: Major capsid protein L1



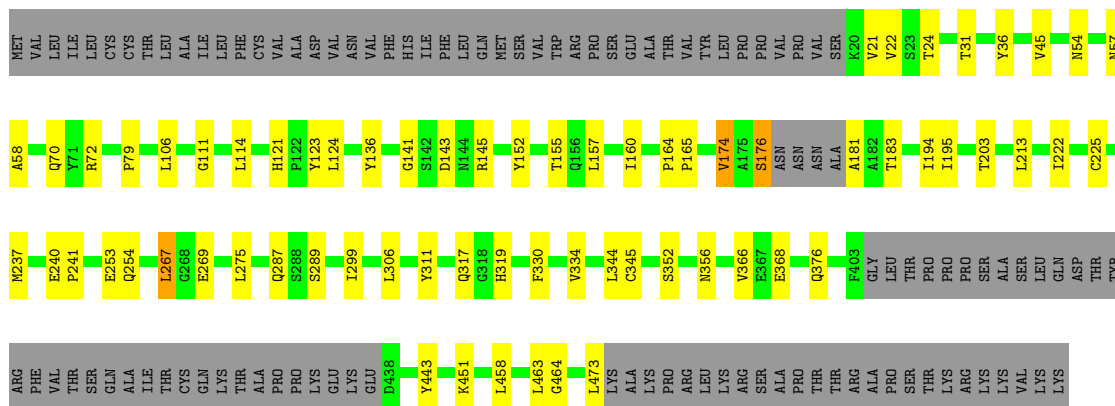
● Molecule 1: Major capsid protein L1



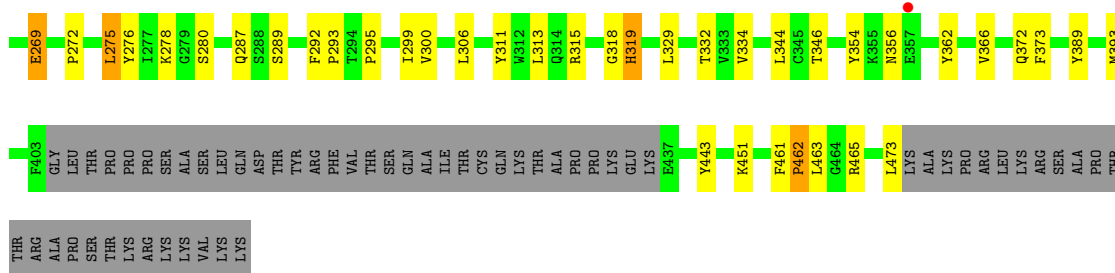
• Molecule 1: Major capsid protein L1



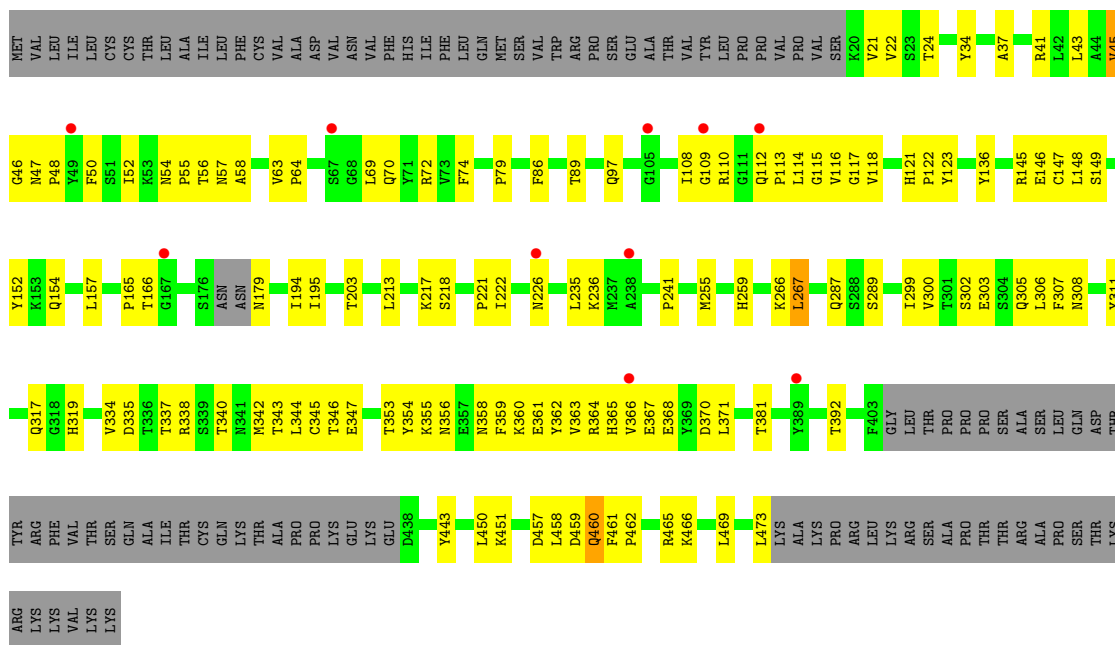
• Molecule 1: Major capsid protein L1



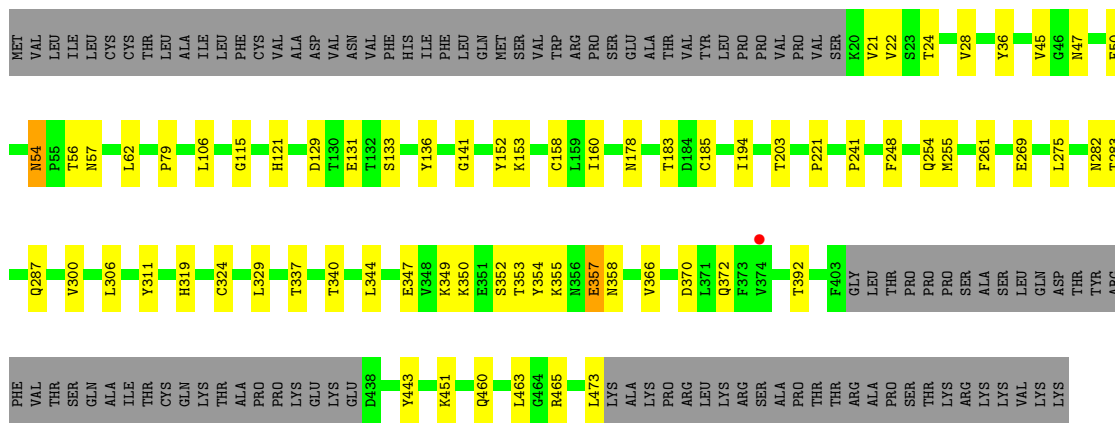
• Molecule 1: Major capsid protein L1



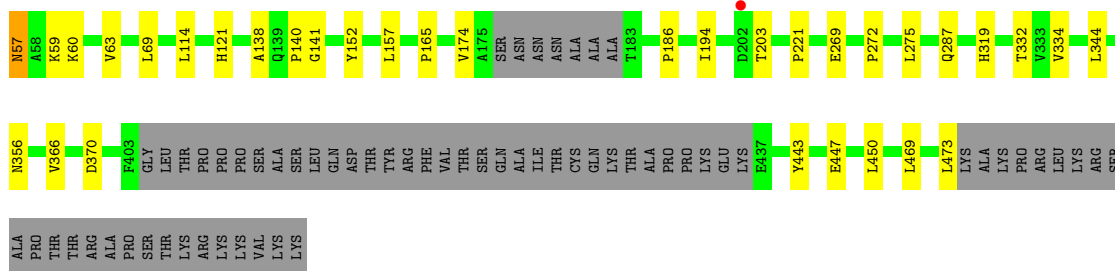
• Molecule 1: Major capsid protein L1



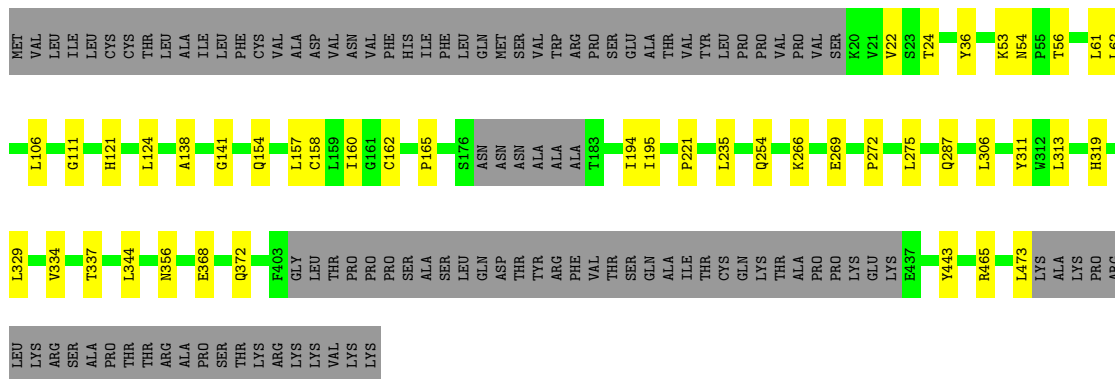
• Molecule 1: Major capsid protein L1



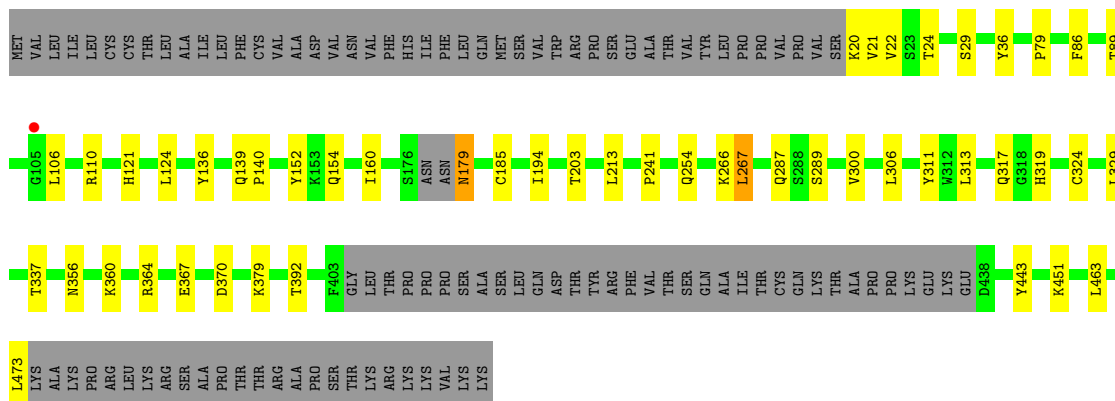
• Molecule 1: Major capsid protein L1



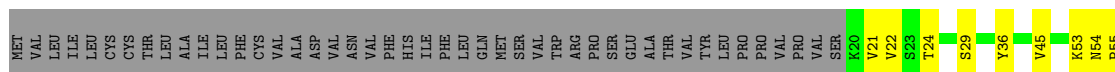
• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	136.54Å 209.76Å 212.63Å 60.50° 85.07° 90.12°	Depositor
Resolution (Å)	41.55 – 3.50 41.55 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (41.55-3.50) 95.7 (41.55-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.315 , 0.340 0.314 , 0.339	Depositor DCC
R_{free} test set	12559 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtrriage
Anisotropy	0.662	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 82.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.135 for -h,k,k-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	133128	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/3442	0.36	0/4670
1	B	0.12	0/3396	0.32	0/4605
1	C	0.13	0/3413	0.33	0/4627
1	D	0.13	0/3418	0.34	0/4634
1	E	0.16	0/3395	0.39	0/4604
1	F	0.12	0/3416	0.36	2/4631 (0.0%)
1	G	0.12	0/3405	0.32	0/4616
1	H	0.11	0/3411	0.32	0/4624
1	I	0.10	0/3425	0.33	0/4644
1	J	0.11	0/3442	0.33	0/4669
1	K	0.14	0/3407	0.37	0/4620
1	L	0.13	0/3405	0.34	0/4616
1	M	0.13	0/3411	0.33	0/4624
1	N	0.12	0/3412	0.33	0/4626
1	O	0.13	0/3442	0.34	0/4669
1	P	0.12	0/3407	0.37	2/4620 (0.0%)
1	Q	0.12	0/3405	0.33	0/4616
1	R	0.12	0/3411	0.34	0/4624
1	S	0.12	0/3425	0.33	0/4644
1	T	0.13	0/3442	0.33	0/4669
1	U	0.12	0/3400	0.34	0/4610
1	V	0.11	0/3405	0.32	0/4616
1	W	0.16	0/3411	0.42	0/4624
1	X	0.17	0/3425	0.42	0/4644
1	Y	0.12	0/3442	0.34	0/4669
1	Z	0.12	0/3407	0.36	2/4620 (0.0%)
1	a	0.11	0/3405	0.31	0/4616
1	b	0.11	0/3411	0.31	0/4624
1	c	0.10	0/3425	0.32	0/4644
1	d	0.11	0/3442	0.33	0/4669
1	e	0.16	0/3416	0.43	2/4631 (0.0%)
1	f	0.14	0/3405	0.37	0/4616
1	g	0.12	0/3411	0.34	0/4624
1	h	0.12	0/3425	0.33	0/4644

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.14	0/3442	0.36	0/4669
1	j	0.14	0/3407	0.34	0/4620
1	k	0.12	0/3405	0.32	0/4616
1	l	0.11	0/3411	0.31	0/4624
1	m	0.12	0/3425	0.33	0/4644
1	n	0.12	0/3442	0.33	0/4669
All	All	0.13	0/136692	0.34	8/185345 (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.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	e	24	THR	CA-C-N	5.89	132.78	121.54
1	e	24	THR	C-N-CA	5.89	132.78	121.54
1	P	23	SER	CA-C-N	5.84	132.69	121.54
1	P	23	SER	C-N-CA	5.84	132.69	121.54
1	F	24	THR	CA-C-N	5.11	131.29	121.54

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 [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	3352	0	3233	42	0
1	B	3307	0	3194	39	0
1	C	3327	0	3213	29	0
1	D	3329	0	3218	39	0
1	E	3307	0	3188	41	0
1	F	3327	0	3217	48	0
1	G	3316	0	3207	39	0
1	H	3322	0	3212	37	0
1	I	3336	0	3227	42	0
1	J	3352	0	3240	43	0
1	K	3318	0	3204	52	0
1	L	3316	0	3207	36	0
1	M	3322	0	3212	43	0
1	N	3323	0	3216	46	0
1	O	3352	0	3240	46	0
1	P	3318	0	3204	29	0
1	Q	3316	0	3207	32	0
1	R	3322	0	3212	32	0
1	S	3336	0	3227	35	0
1	T	3352	0	3240	41	0
1	U	3311	0	3195	64	0
1	V	3316	0	3207	42	0
1	W	3322	0	3212	139	0
1	X	3336	0	3227	142	1
1	Y	3352	0	3240	53	0
1	Z	3318	0	3204	49	0
1	a	3316	0	3207	42	0
1	b	3322	0	3212	33	0
1	c	3336	0	3227	37	0
1	d	3352	0	3240	45	0
1	e	3327	0	3217	120	0
1	f	3316	0	3207	102	0
1	g	3322	0	3212	47	1
1	h	3336	0	3227	52	0
1	i	3352	0	3240	68	0
1	j	3318	0	3204	39	0
1	k	3316	0	3207	27	0
1	l	3322	0	3212	26	0
1	m	3336	0	3227	32	0
1	n	3352	0	3240	35	0
All	All	133128	0	128682	1532	1

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 6.

The worst 5 of 1532 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:235:LEU:HD21	1:X:109:GLY:HA3	1.34	1.08
1:W:315:ARG:HD3	1:X:469:LEU:HD11	1.43	1.00
1:U:280:SER:HB3	1:X:353:THR:HB	1.47	0.94
1:f:280:SER:HB3	1:g:353:THR:HB	1.48	0.94
1:e:122:PRO:HD3	1:f:289:SER:HB3	1.47	0.93

All (1) 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:X:89:THR:OG1	1:g:56:THR:OG1[1_655]	2.10	0.10

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	417/524 (80%)	399 (96%)	17 (4%)	1 (0%)	43	74
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%)	43	74
1	F	411/524 (78%)	388 (94%)	20 (5%)	3 (1%)	18	51
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%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	57
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%)	24	57
1	V	409/524 (78%)	390 (95%)	19 (5%)	0	100	100
1	W	410/524 (78%)	392 (96%)	17 (4%)	1 (0%)	43	74
1	X	413/524 (79%)	394 (95%)	19 (5%)	0	100	100
1	Y	417/524 (80%)	399 (96%)	17 (4%)	1 (0%)	43	74
1	Z	410/524 (78%)	389 (95%)	17 (4%)	4 (1%)	12	44
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%)	12	44
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%)	43	74
1	j	410/524 (78%)	390 (95%)	19 (5%)	1 (0%)	43	74
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%)	43	74
All	All	16467/20960 (79%)	15714 (95%)	729 (4%)	24 (0%)	48	79

5 of 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

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/466 (80%)	369 (99%)	4 (1%)	65	74
1	B	369/466 (79%)	368 (100%)	1 (0%)	86	83
1	C	371/466 (80%)	369 (100%)	2 (0%)	81	80
1	D	372/466 (80%)	369 (99%)	3 (1%)	73	77
1	E	368/466 (79%)	366 (100%)	2 (0%)	81	80
1	F	371/466 (80%)	368 (99%)	3 (1%)	73	77
1	G	370/466 (79%)	368 (100%)	2 (0%)	81	80
1	H	371/466 (80%)	368 (99%)	3 (1%)	73	77
1	I	371/466 (80%)	365 (98%)	6 (2%)	55	70
1	J	373/466 (80%)	366 (98%)	7 (2%)	50	68
1	K	370/466 (79%)	368 (100%)	2 (0%)	81	80
1	L	370/466 (79%)	367 (99%)	3 (1%)	73	77
1	M	371/466 (80%)	365 (98%)	6 (2%)	55	70
1	N	370/466 (79%)	364 (98%)	6 (2%)	55	70
1	O	373/466 (80%)	365 (98%)	8 (2%)	47	66
1	P	370/466 (79%)	365 (99%)	5 (1%)	59	71
1	Q	370/466 (79%)	368 (100%)	2 (0%)	81	80
1	R	371/466 (80%)	367 (99%)	4 (1%)	65	74
1	S	371/466 (80%)	365 (98%)	6 (2%)	55	70
1	T	373/466 (80%)	367 (98%)	6 (2%)	55	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	369/466 (79%)	367 (100%)	2 (0%)	81	80
1	V	370/466 (79%)	368 (100%)	2 (0%)	81	80
1	W	371/466 (80%)	364 (98%)	7 (2%)	50	68
1	X	371/466 (80%)	364 (98%)	7 (2%)	50	68
1	Y	373/466 (80%)	366 (98%)	7 (2%)	50	68
1	Z	370/466 (79%)	367 (99%)	3 (1%)	73	77
1	a	370/466 (79%)	368 (100%)	2 (0%)	81	80
1	b	371/466 (80%)	367 (99%)	4 (1%)	65	74
1	c	371/466 (80%)	367 (99%)	4 (1%)	65	74
1	d	373/466 (80%)	369 (99%)	4 (1%)	65	74
1	e	371/466 (80%)	365 (98%)	6 (2%)	55	70
1	f	370/466 (79%)	366 (99%)	4 (1%)	65	74
1	g	371/466 (80%)	366 (99%)	5 (1%)	61	72
1	h	371/466 (80%)	366 (99%)	5 (1%)	61	72
1	i	373/466 (80%)	367 (98%)	6 (2%)	55	70
1	j	370/466 (79%)	366 (99%)	4 (1%)	65	74
1	k	370/466 (79%)	364 (98%)	6 (2%)	55	70
1	l	371/466 (80%)	367 (99%)	4 (1%)	65	74
1	m	371/466 (80%)	366 (99%)	5 (1%)	61	72
1	n	373/466 (80%)	365 (98%)	8 (2%)	47	66
All	All	14838/18640 (80%)	14662 (99%)	176 (1%)	65	73

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	22	VAL
1	i	22	VAL
1	d	22	VAL
1	f	269	GLU
1	j	27	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	c	144	ASN
1	h	179	ASN
1	c	254	GLN
1	e	154	GLN
1	k	57	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	420/524 (80%)	-0.53	0 100 100	22, 48, 99, 169	1 (0%)
1	B	413/524 (78%)	-0.68	0 100 100	24, 49, 90, 149	1 (0%)
1	C	416/524 (79%)	-0.52	0 100 100	34, 58, 102, 156	0
1	D	416/524 (79%)	-0.59	0 100 100	24, 52, 91, 154	1 (0%)
1	E	414/524 (79%)	-0.61	0 100 100	32, 57, 94, 177	1 (0%)
1	F	416/524 (79%)	-0.05	1 (0%) 91 82	71, 120, 165, 282	1 (0%)
1	G	414/524 (79%)	-0.02	1 (0%) 91 82	61, 105, 154, 200	1 (0%)
1	H	415/524 (79%)	-0.07	3 (0%) 84 63	87, 148, 186, 252	1 (0%)
1	I	418/524 (79%)	-0.10	0 100 100	102, 163, 204, 283	1 (0%)
1	J	420/524 (80%)	0.33	7 (1%) 69 43	79, 136, 180, 339	1 (0%)
1	K	415/524 (79%)	-0.57	0 100 100	26, 50, 91, 204	1 (0%)
1	L	414/524 (79%)	-0.65	0 100 100	18, 48, 101, 157	1 (0%)
1	M	415/524 (79%)	-0.67	0 100 100	16, 44, 81, 164	1 (0%)
1	N	416/524 (79%)	-0.61	0 100 100	28, 51, 97, 218	1 (0%)
1	O	420/524 (80%)	-0.58	0 100 100	22, 46, 90, 171	1 (0%)
1	P	415/524 (79%)	0.11	0 100 100	62, 93, 131, 186	1 (0%)
1	Q	414/524 (79%)	0.06	1 (0%) 91 82	57, 90, 133, 205	1 (0%)
1	R	415/524 (79%)	0.26	2 (0%) 87 68	46, 92, 120, 198	1 (0%)
1	S	418/524 (79%)	-0.14	0 100 100	44, 76, 119, 226	1 (0%)
1	T	420/524 (80%)	-0.01	0 100 100	38, 77, 105, 180	1 (0%)
1	U	414/524 (79%)	0.42	6 (1%) 73 48	82, 151, 186, 304	1 (0%)
1	V	414/524 (79%)	0.16	2 (0%) 87 68	67, 149, 192, 215	1 (0%)
1	W	415/524 (79%)	0.18	10 (2%) 59 35	91, 139, 189, 260	1 (0%)
1	X	418/524 (79%)	0.11	10 (2%) 59 35	77, 148, 189, 242	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	420/524 (80%)	-0.22	1 (0%) 91 82	76, 122, 161, 378	1 (0%)
1	Z	415/524 (79%)	0.29	6 (1%) 73 48	83, 146, 184, 281	1 (0%)
1	a	414/524 (79%)	0.27	5 (1%) 76 52	94, 152, 178, 196	1 (0%)
1	b	415/524 (79%)	0.20	6 (1%) 73 48	89, 148, 177, 270	1 (0%)
1	c	418/524 (79%)	-0.01	5 (1%) 76 52	81, 146, 182, 291	1 (0%)
1	d	420/524 (80%)	-0.09	0 100 100	93, 159, 202, 390	1 (0%)
1	e	416/524 (79%)	0.02	3 (0%) 84 63	66, 126, 167, 256	1 (0%)
1	f	414/524 (79%)	-0.28	0 100 100	26, 85, 168, 212	1 (0%)
1	g	415/524 (79%)	0.05	7 (1%) 69 43	80, 126, 156, 226	1 (0%)
1	h	418/524 (79%)	-0.13	1 (0%) 91 82	75, 123, 167, 227	1 (0%)
1	i	420/524 (80%)	0.17	3 (0%) 84 63	68, 132, 185, 335	1 (0%)
1	j	415/524 (79%)	0.03	4 (0%) 79 56	44, 72, 109, 166	1 (0%)
1	k	414/524 (79%)	-0.14	1 (0%) 91 82	51, 82, 118, 172	1 (0%)
1	l	415/524 (79%)	-0.05	0 100 100	49, 82, 124, 221	1 (0%)
1	m	418/524 (79%)	-0.09	1 (0%) 91 82	46, 82, 116, 194	1 (0%)
1	n	420/524 (80%)	-0.20	0 100 100	52, 81, 132, 351	1 (0%)
All	All	16652/20960 (79%)	-0.12	86 (0%) 87 68	16, 102, 174, 390	39 (0%)

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	214	GLN	3.8
1	H	220	VAL	3.4
1	X	366	VAL	3.3
1	a	171	GLY	3.2
1	g	225	CYS	3.2

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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.