wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 05:32 AM EDT

PDB ID	:	2R5J
Title	:	Pentamer Structure of Major Capsid protein L1 of Human Papilloma Virus Type 35
Authors	:	Bishop, B.; Dasgupta, J.; Chen, X.S.
Deposited on	:	2007-09-03
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

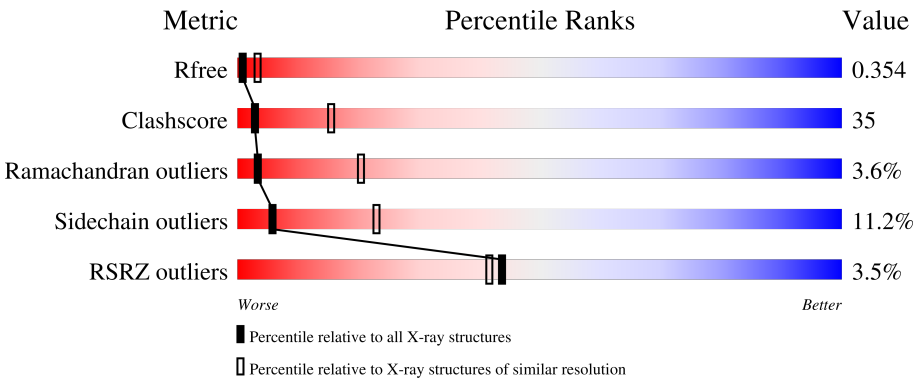
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	423	2%, 36%, 39%, 22%, • •
1	B	423	2%, 34%, 40%, 20%, • •
1	C	423	3%, 30%, 41%, 23%, 5%, •
1	D	423	4%, 35%, 40%, 21%, • •
1	E	423	3%, 30%, 44%, 22%, • •

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Mol	Chain	Length	Quality of chain
1	F	423	5% 34% 39% 22%
1	G	423	2% 33% 44% 20%
1	H	423	4% 34% 44% 17%
1	I	423	3% 30% 41% 24%
1	J	423	3% 33% 40% 23%
1	K	423	5% 28% 45% 23%
1	L	423	3% 34% 41% 22%
1	M	423	4% 29% 45% 22%
1	N	423	3% 33% 44% 19%
1	O	423	6% 30% 44% 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 49350 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	417	3290	2089	551	630	20	0	0	0
1	B	417	3290	2089	551	630	20	0	0	0
1	C	417	3290	2089	551	630	20	0	0	0
1	D	417	3290	2089	551	630	20	0	0	0
1	E	417	3290	2089	551	630	20	0	0	0
1	F	417	3290	2089	551	630	20	0	0	0
1	G	417	3290	2089	551	630	20	0	0	0
1	H	417	3290	2089	551	630	20	0	0	0
1	I	417	3290	2089	551	630	20	0	0	0
1	J	417	3290	2089	551	630	20	0	0	0
1	K	417	3290	2089	551	630	20	0	0	0
1	L	417	3290	2089	551	630	20	0	0	0
1	M	417	3290	2089	551	630	20	0	0	0
1	N	417	3290	2089	551	630	20	0	0	0
1	O	417	3290	2089	551	630	20	0	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP P27232
A	175	SER	CYS	engineered mutation	UNP P27232
A	402	GLY	-	linker	UNP P27232
A	403	GLY	-	linker	UNP P27232
A	404	SER	-	linker	UNP P27232
A	405	GLY	-	linker	UNP P27232
A	406	GLY	-	linker	UNP P27232
B	20	ALA	-	expression tag	UNP P27232
B	175	SER	CYS	engineered mutation	UNP P27232
B	402	GLY	-	linker	UNP P27232
B	403	GLY	-	linker	UNP P27232
B	404	SER	-	linker	UNP P27232
B	405	GLY	-	linker	UNP P27232
B	406	GLY	-	linker	UNP P27232
C	20	ALA	-	expression tag	UNP P27232
C	175	SER	CYS	engineered mutation	UNP P27232
C	402	GLY	-	linker	UNP P27232
C	403	GLY	-	linker	UNP P27232
C	404	SER	-	linker	UNP P27232
C	405	GLY	-	linker	UNP P27232
C	406	GLY	-	linker	UNP P27232
D	20	ALA	-	expression tag	UNP P27232
D	175	SER	CYS	engineered mutation	UNP P27232
D	402	GLY	-	linker	UNP P27232
D	403	GLY	-	linker	UNP P27232
D	404	SER	-	linker	UNP P27232
D	405	GLY	-	linker	UNP P27232
D	406	GLY	-	linker	UNP P27232
E	20	ALA	-	expression tag	UNP P27232
E	175	SER	CYS	engineered mutation	UNP P27232
E	402	GLY	-	linker	UNP P27232
E	403	GLY	-	linker	UNP P27232
E	404	SER	-	linker	UNP P27232
E	405	GLY	-	linker	UNP P27232
E	406	GLY	-	linker	UNP P27232
F	20	ALA	-	expression tag	UNP P27232
F	175	SER	CYS	engineered mutation	UNP P27232
F	402	GLY	-	linker	UNP P27232
F	403	GLY	-	linker	UNP P27232
F	404	SER	-	linker	UNP P27232
F	405	GLY	-	linker	UNP P27232
F	406	GLY	-	linker	UNP P27232
G	20	ALA	-	expression tag	UNP P27232

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Chain	Residue	Modelled	Actual	Comment	Reference
G	175	SER	CYS	engineered mutation	UNP P27232
G	402	GLY	-	linker	UNP P27232
G	403	GLY	-	linker	UNP P27232
G	404	SER	-	linker	UNP P27232
G	405	GLY	-	linker	UNP P27232
G	406	GLY	-	linker	UNP P27232
H	20	ALA	-	expression tag	UNP P27232
H	175	SER	CYS	engineered mutation	UNP P27232
H	402	GLY	-	linker	UNP P27232
H	403	GLY	-	linker	UNP P27232
H	404	SER	-	linker	UNP P27232
H	405	GLY	-	linker	UNP P27232
H	406	GLY	-	linker	UNP P27232
I	20	ALA	-	expression tag	UNP P27232
I	175	SER	CYS	engineered mutation	UNP P27232
I	402	GLY	-	linker	UNP P27232
I	403	GLY	-	linker	UNP P27232
I	404	SER	-	linker	UNP P27232
I	405	GLY	-	linker	UNP P27232
I	406	GLY	-	linker	UNP P27232
J	20	ALA	-	expression tag	UNP P27232
J	175	SER	CYS	engineered mutation	UNP P27232
J	402	GLY	-	linker	UNP P27232
J	403	GLY	-	linker	UNP P27232
J	404	SER	-	linker	UNP P27232
J	405	GLY	-	linker	UNP P27232
J	406	GLY	-	linker	UNP P27232
K	20	ALA	-	expression tag	UNP P27232
K	175	SER	CYS	engineered mutation	UNP P27232
K	402	GLY	-	linker	UNP P27232
K	403	GLY	-	linker	UNP P27232
K	404	SER	-	linker	UNP P27232
K	405	GLY	-	linker	UNP P27232
K	406	GLY	-	linker	UNP P27232
L	20	ALA	-	expression tag	UNP P27232
L	175	SER	CYS	engineered mutation	UNP P27232
L	402	GLY	-	linker	UNP P27232
L	403	GLY	-	linker	UNP P27232
L	404	SER	-	linker	UNP P27232
L	405	GLY	-	linker	UNP P27232
L	406	GLY	-	linker	UNP P27232
M	20	ALA	-	expression tag	UNP P27232

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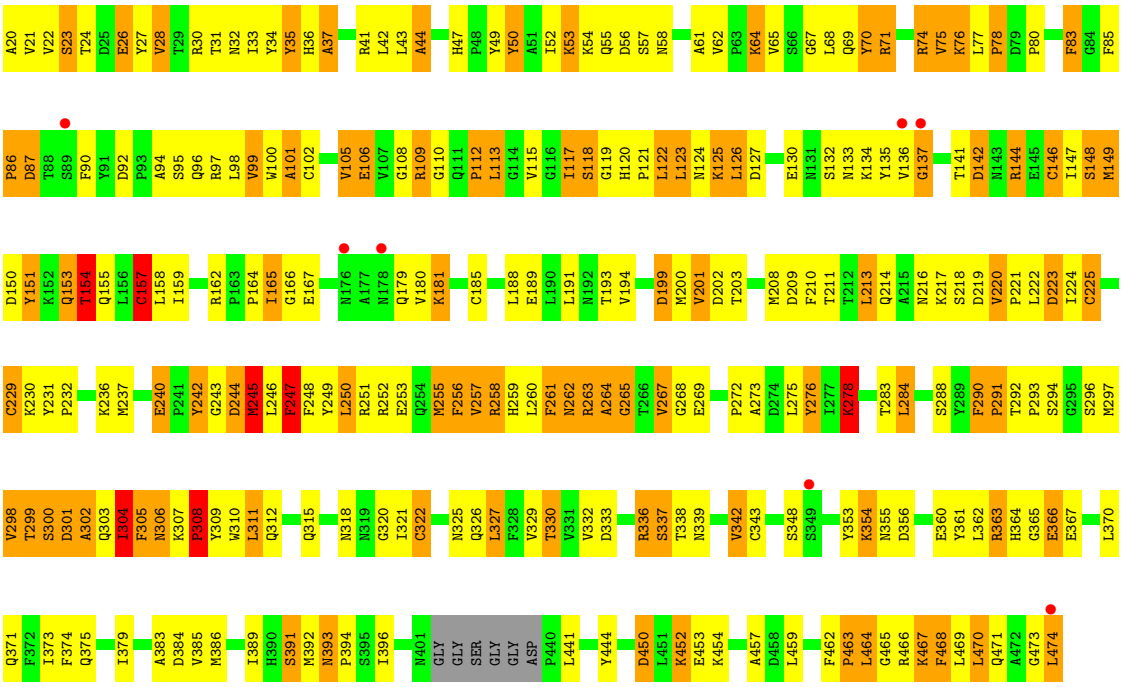
Chain	Residue	Modelled	Actual	Comment	Reference
M	175	SER	CYS	engineered mutation	UNP P27232
M	402	GLY	-	linker	UNP P27232
M	403	GLY	-	linker	UNP P27232
M	404	SER	-	linker	UNP P27232
M	405	GLY	-	linker	UNP P27232
M	406	GLY	-	linker	UNP P27232
N	20	ALA	-	expression tag	UNP P27232
N	175	SER	CYS	engineered mutation	UNP P27232
N	402	GLY	-	linker	UNP P27232
N	403	GLY	-	linker	UNP P27232
N	404	SER	-	linker	UNP P27232
N	405	GLY	-	linker	UNP P27232
N	406	GLY	-	linker	UNP P27232
O	20	ALA	-	expression tag	UNP P27232
O	175	SER	CYS	engineered mutation	UNP P27232
O	402	GLY	-	linker	UNP P27232
O	403	GLY	-	linker	UNP P27232
O	404	SER	-	linker	UNP P27232
O	405	GLY	-	linker	UNP P27232
O	406	GLY	-	linker	UNP P27232

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.

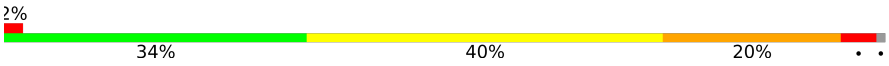
• Molecule 1: Major capsid protein L1

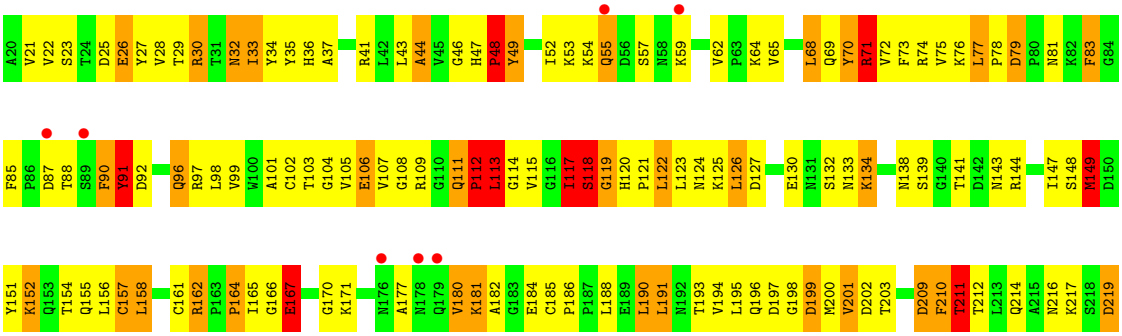
Chain A:

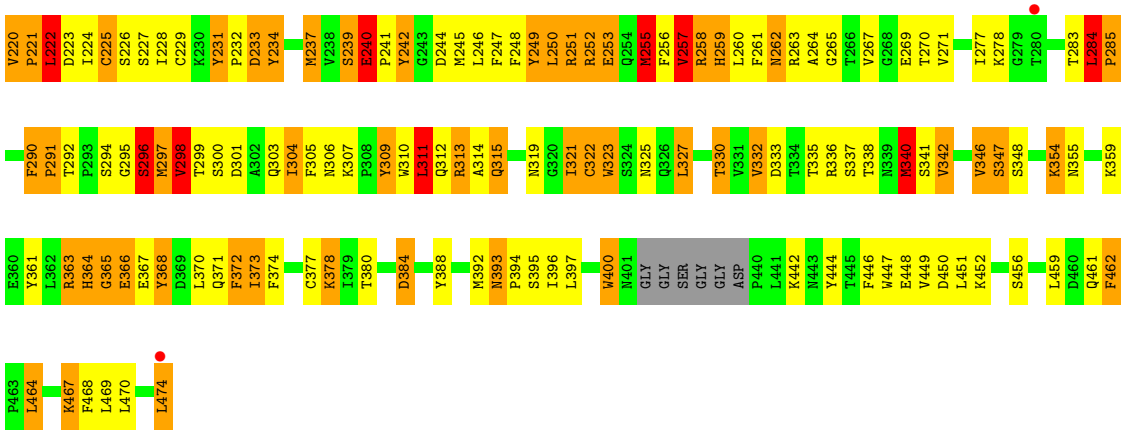


• Molecule 1: Major capsid protein L1

Chain B:

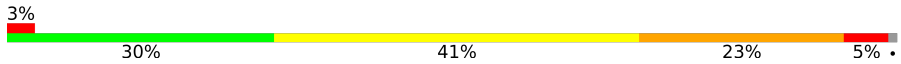


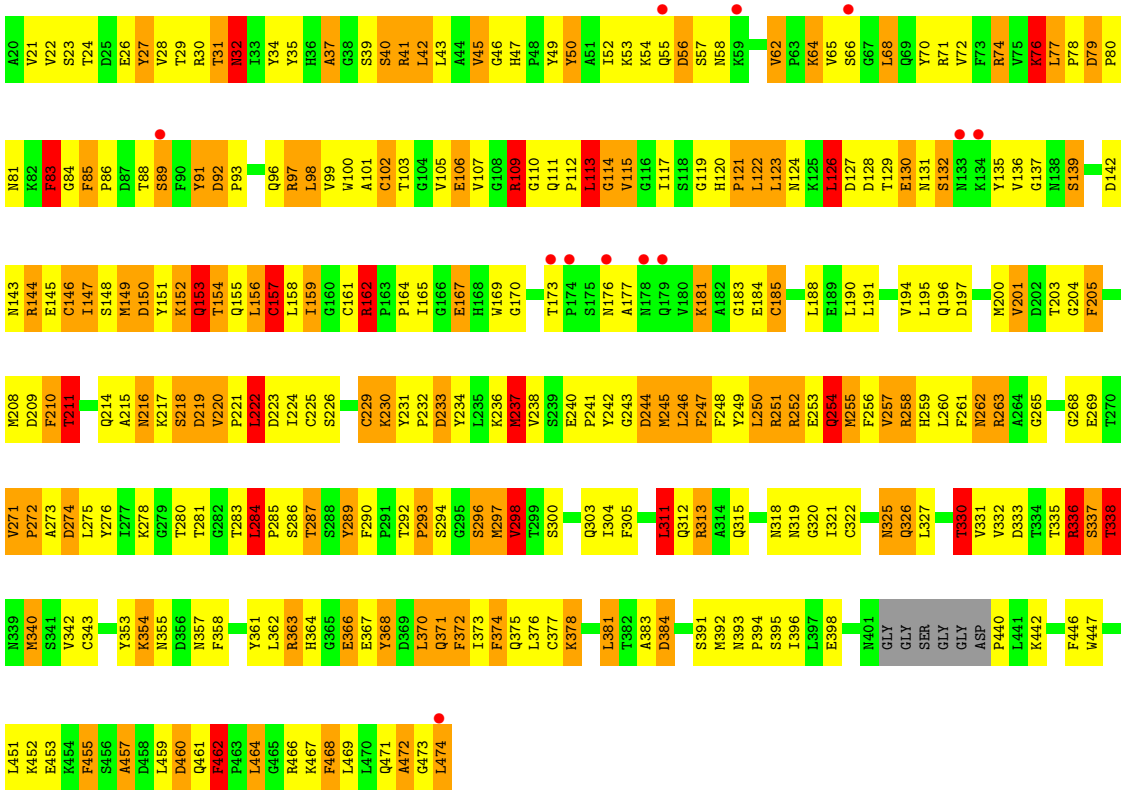




• Molecule 1: Major capsid protein L1

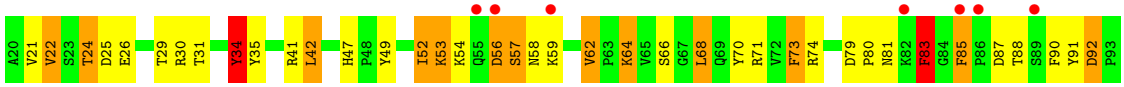
Chain C:

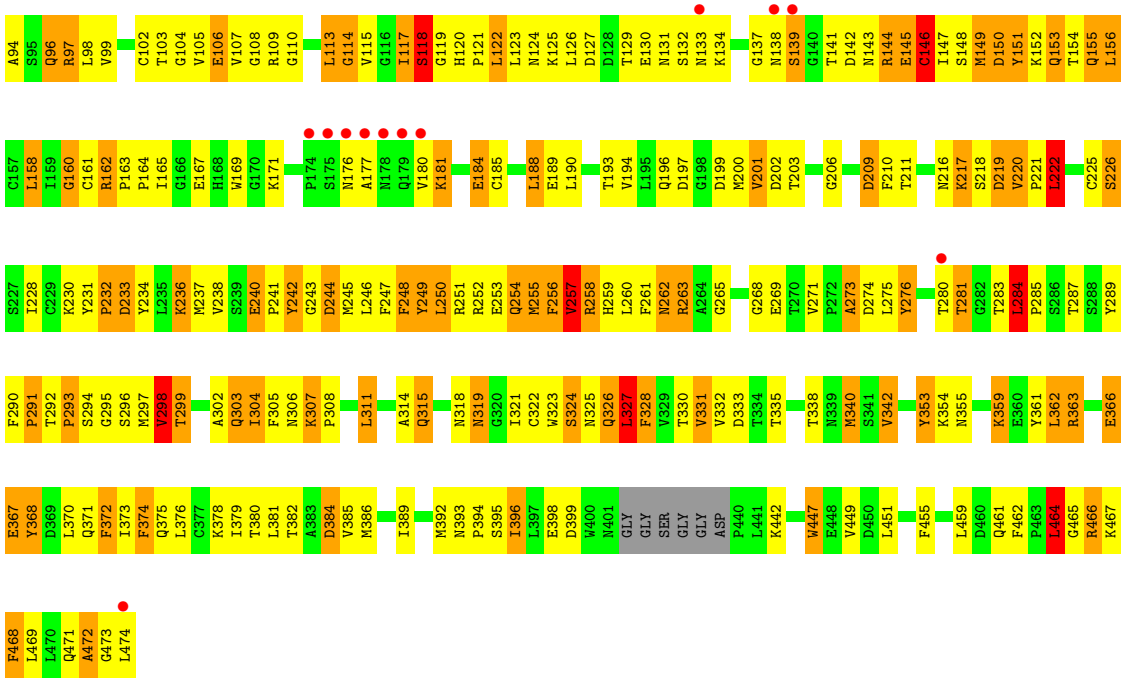




• Molecule 1: Major capsid protein L1

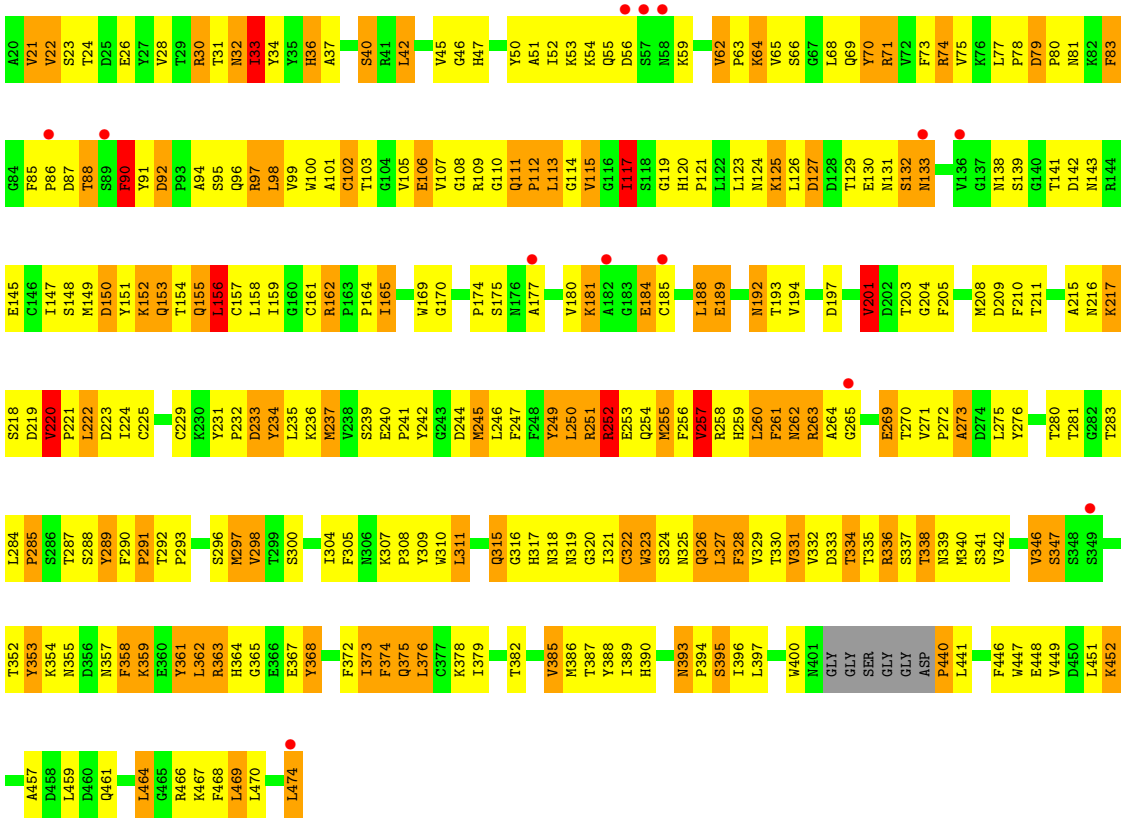
Chain D:





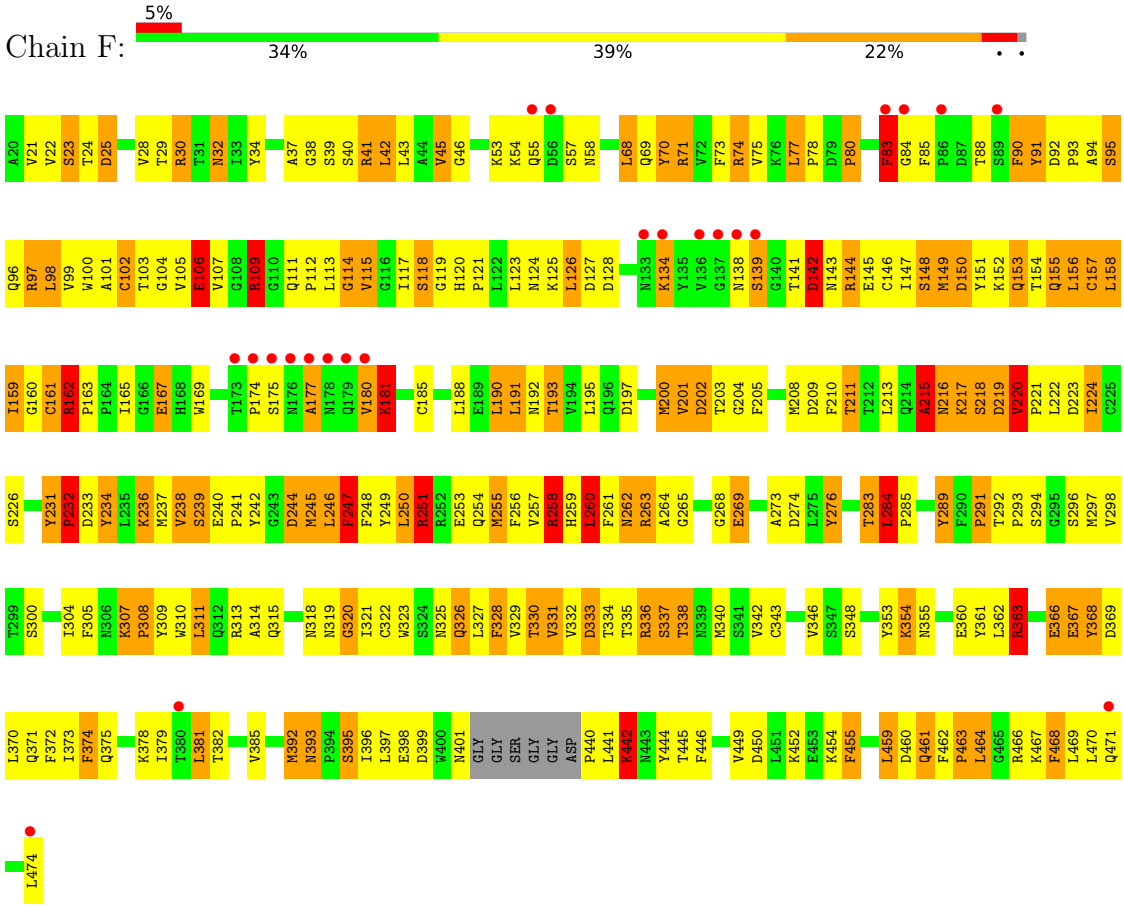
• Molecule 1: Major capsid protein L1

Chain E: 3% 30% 44% 22%



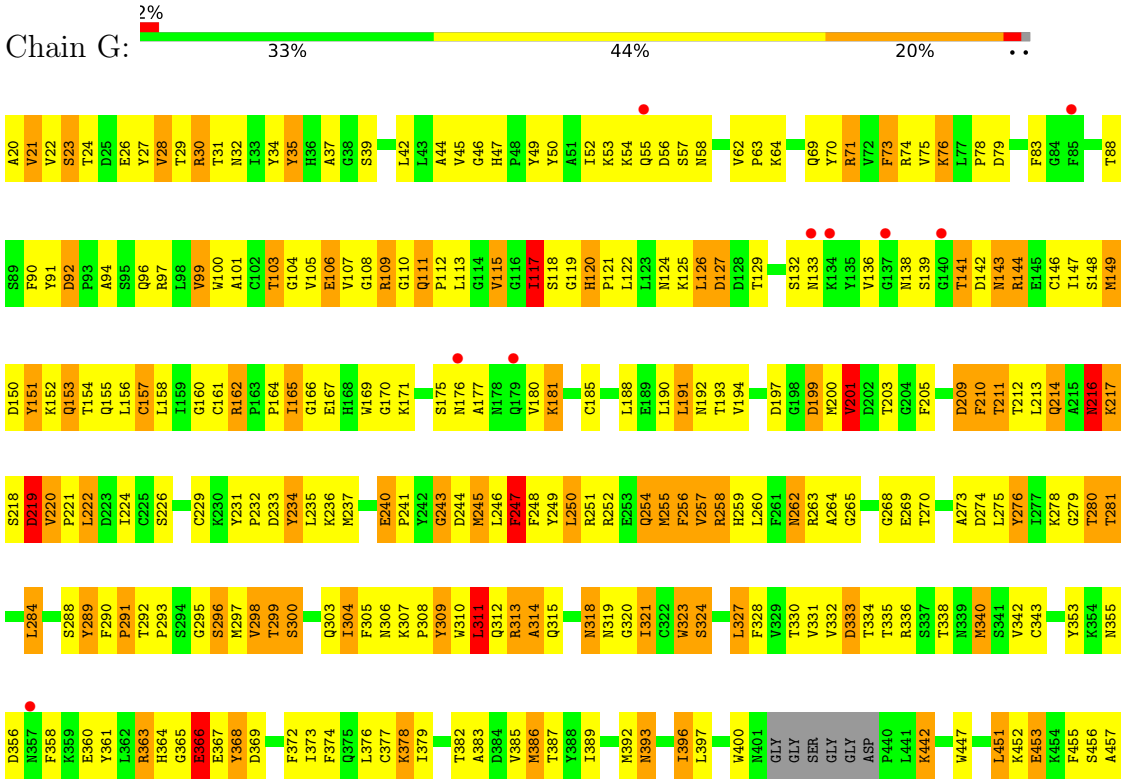
• Molecule 1: Major capsid protein L1

Chain F:



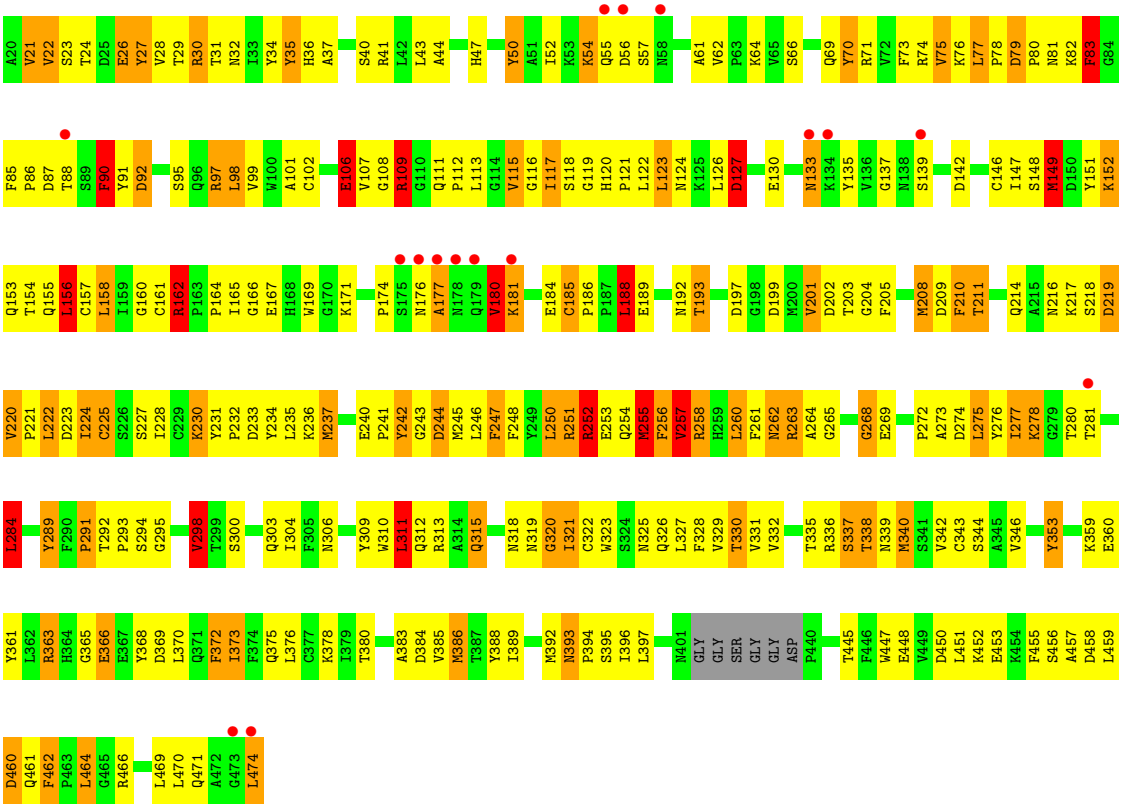
- Molecule 1: Major capsid protein L1

Chain G:



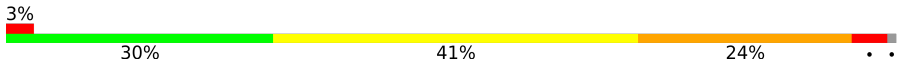
• Molecule 1: Major capsid protein L1

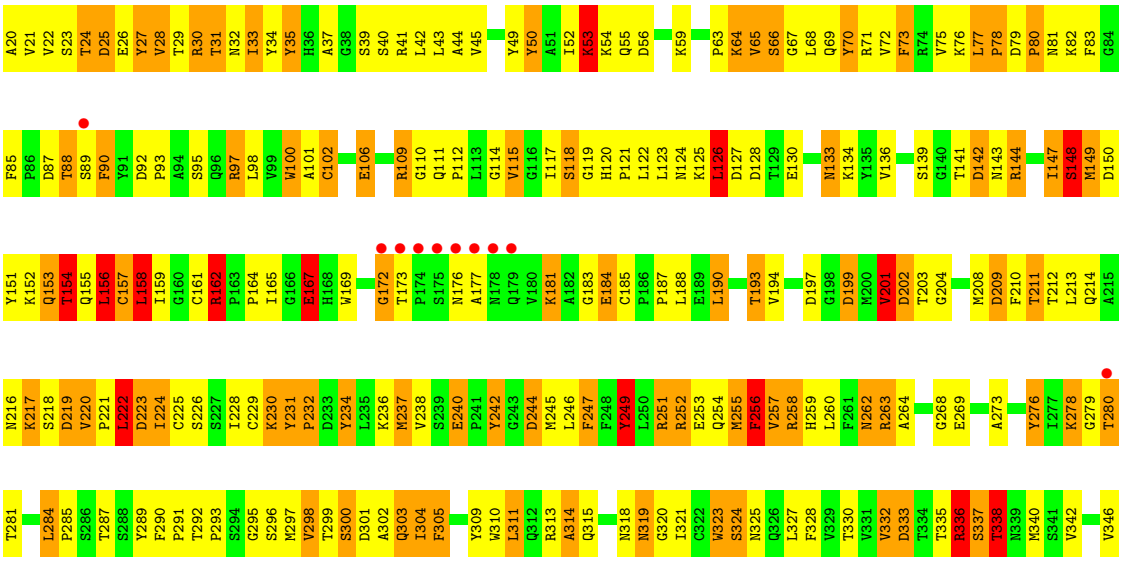
Chain H:

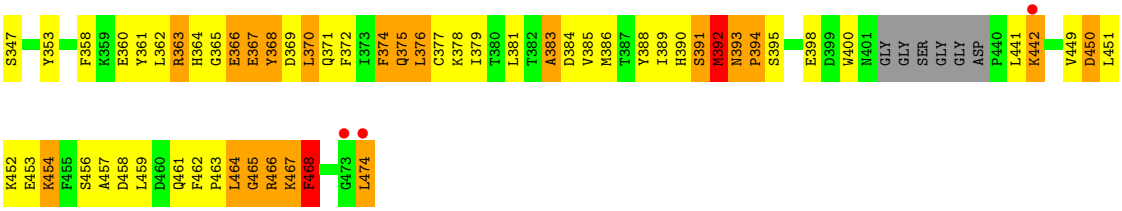


• Molecule 1: Major capsid protein L1

Chain I:

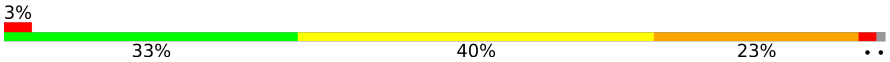


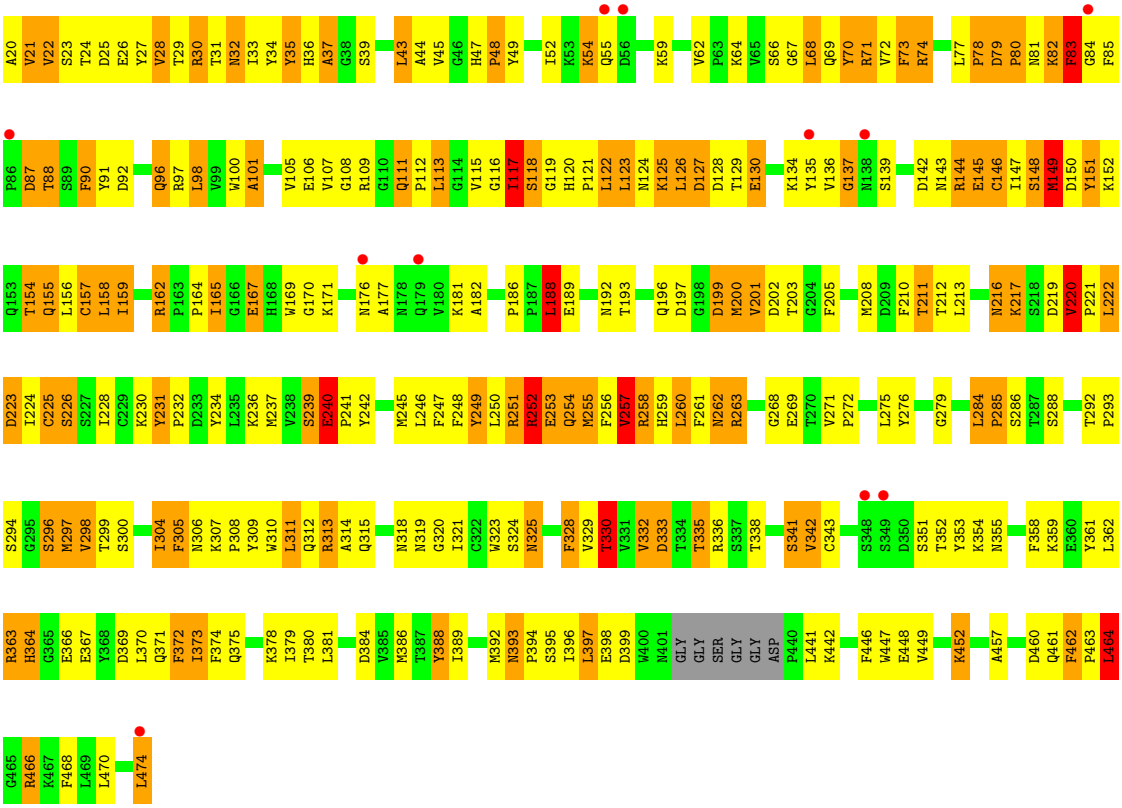




• Molecule 1: Major capsid protein L1

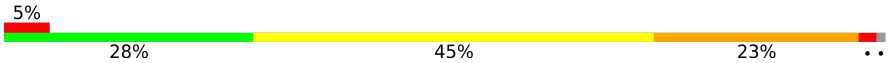
Chain J:

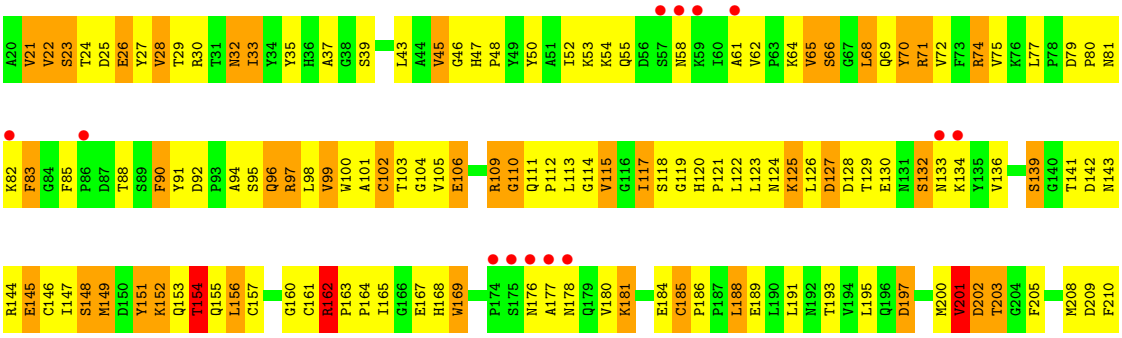


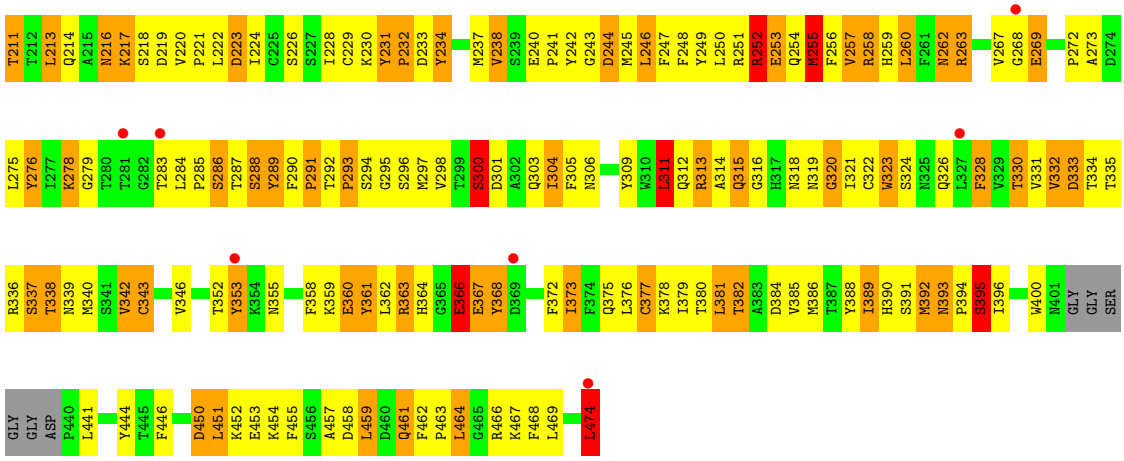


• Molecule 1: Major capsid protein L1

Chain K:

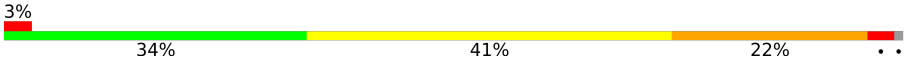


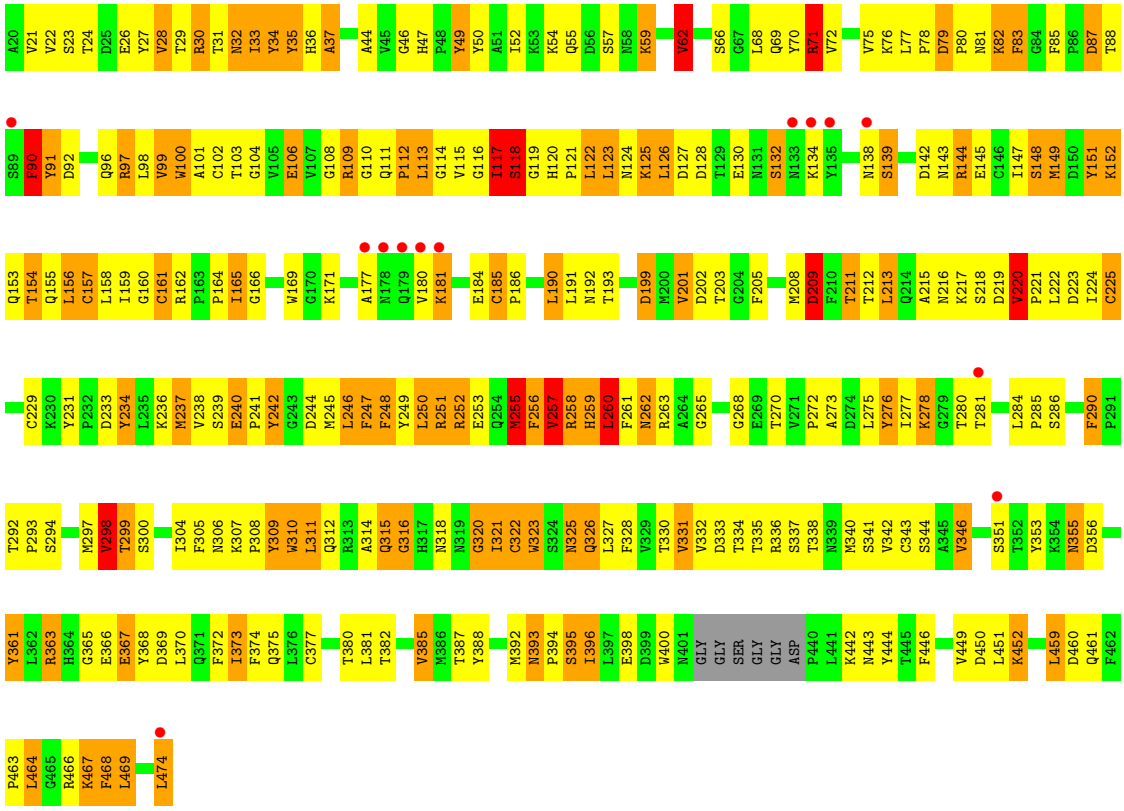




- Molecule 1: Major capsid protein L1

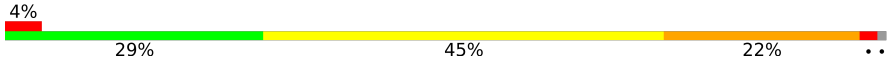
Chain L:

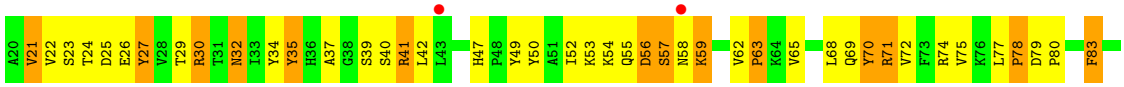


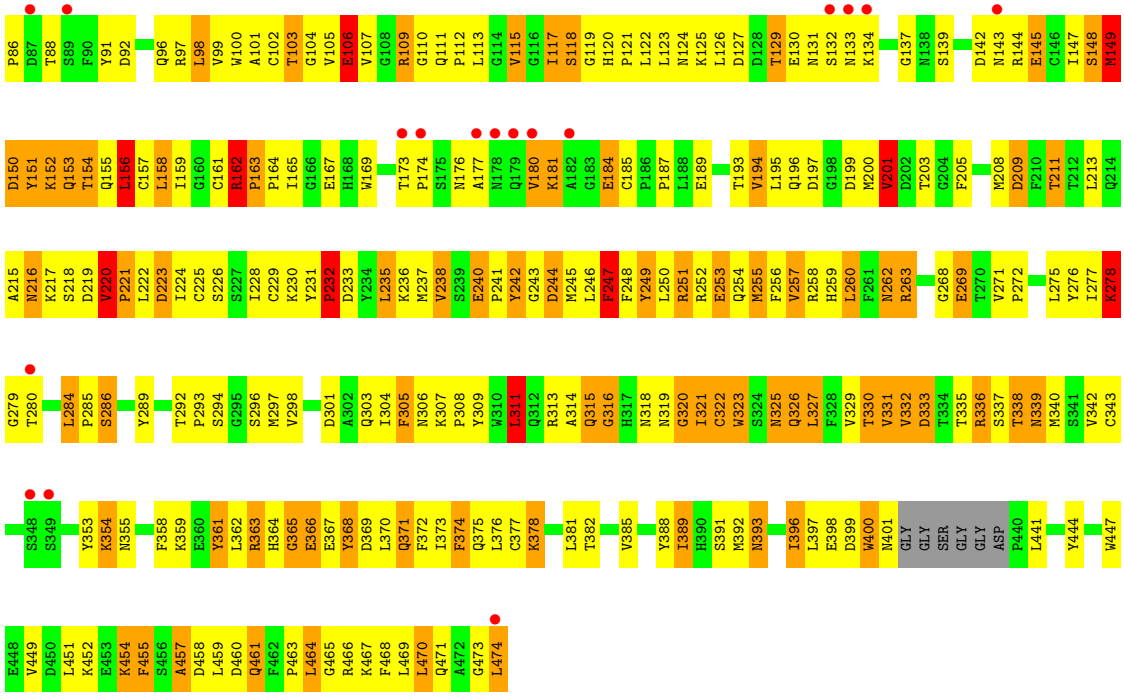


- Molecule 1: Major capsid protein L1

Chain M:

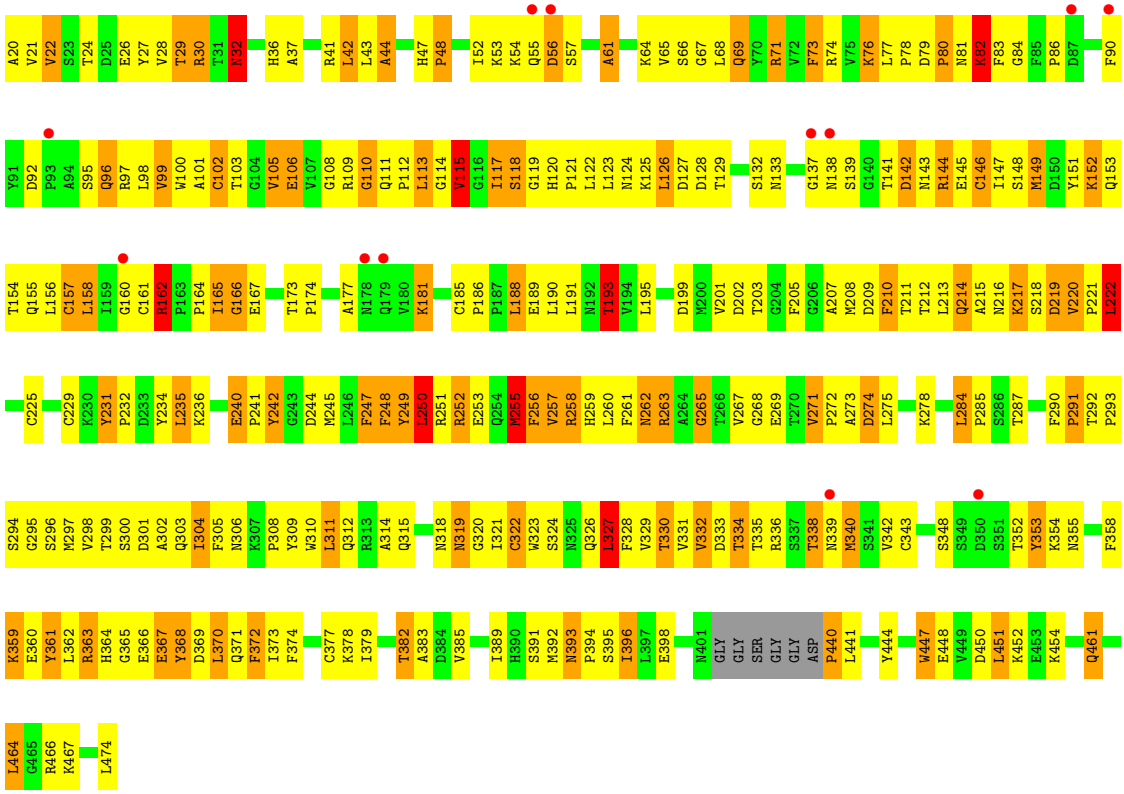






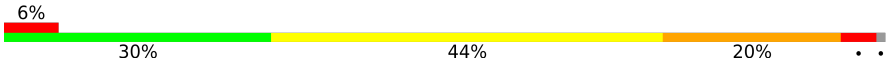
• Molecule 1: Major capsid protein L1

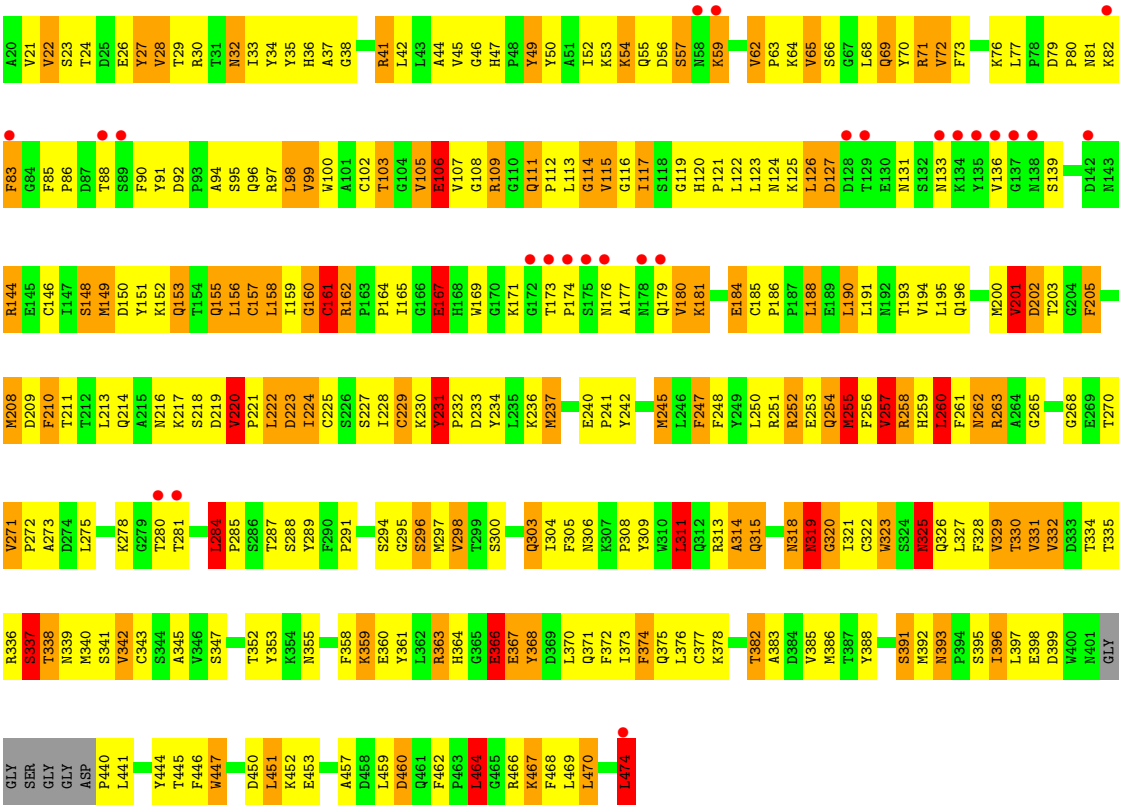
Chain N: 3% 33% 44% 19%



• Molecule 1: Major capsid protein L1

Chain O:


6%
30%
44%
20%


A20 V21 V22 S23 T24 D25 E26 Y27 V28 T29 R30 T31 N32 I33 Y34 Y35 H36 A37 G38 R41 L42 L43 A44 V45 G46 H47 P48 Y49 Y50 A51 I52 K53 K54 Q55 D56 S57 N58 K59 V62 P63 K64 V65 S66 G67 L68 Q69 Y70 R71 V72 F73 K76 L77 P78 D79 P80 N81 K82
F83 G84 F85 P86 D87 T88 S89 F90 Y91 D92 P93 A94 S95 Q96 R97 L98 V99 W100 A101 C102 T103 G104 V105 E106 V107 G108 R109 G110 Q111 P112 L113 G114 V115 G116 I117 S118 G119 H120 P121 L122 L123 N124 K125 L126 D127 D128 T129 E130 N131 S132 N133 K134 Y135 V136 G137 N138 S139 D142 N143
R144 E145 C146 I147 S148 M149 D150 Y151 K152 Q153 T154 Q155 L156 C157 L158 I159 G160 G161 R162 P163 P164 I165 G166 E167 H168 W169 G170 K171 G172 T173 P174 S175 N176 A177 N178 Q179 V180 K181 E184 C185 P186 P187 L188 E189 L190 L191 N192 T193 V194 L195 Q196 M200 V201 D202 T203 G204 F205
M208 D209 F210 T211 T212 L213 Q214 A215 N216 K217 S218 D219 V220 P221 L222 D223 I224 C225 S226 S227 I228 C229 K230 Y231 P232 D233 Y234 L235 K236 M237 E240 P241 Y242 M245 L246 F247 F248 Y249 L250 R251 R252 E253 Q254 M255 F256 V257 R258 H259 L260 F261 N262 R263 A264 G265 G268 E269 T270
V271 P272 A273 D274 L275 K278 G279 T280 T281 L284 P285 S286 T287 S288 Y289 F290 P291 S294 G295 S296 M297 V298 T299 S300 Q303 I304 F305 N306 K307 P308 Y309 W310 L311 Q312 R313 A314 Q315 N318 N319 G320 I321 C322 W323 S324 N325 Q326 L327 F328 V329 T330 V331 V332 D333 T334 T335
R336 S337 T338 N339 M340 S341 V342 C343 S344 A345 V346 S347 T352 Y353 K354 N355 F358 K359 E360 Y361 L362 R363 H364 G365 E366 E367 Y368 D369 L370 Q371 F372 I373 F374 Q375 L376 C377 K378 T382 A383 D384 V385 M386 T387 Y388 S391 M392 N393 P394 S395 I396 L397 E398 D399 W400 N401 GLY
GLY SER GLY GLY ASP P440 L441 Y444 T445 F446 W447 D450 L451 K452 E453 A457 D458 L459 D460 Q461 F462 P463 L464 G465 R466 K467 F468 L469 L470 L474

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	150.41Å 176.61Å 197.07Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 15.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (15.00-3.30) 85.6 (15.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	18.90	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.315 , 0.348 0.319 , 0.354	Depositor DCC
R_{free} test set	7364 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 10.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	49350	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	2.22	117/3373 (3.5%)	1.78	69/4580 (1.5%)
1	B	2.19	117/3373 (3.5%)	1.76	66/4580 (1.4%)
1	C	2.23	114/3373 (3.4%)	1.87	83/4580 (1.8%)
1	D	2.20	100/3373 (3.0%)	1.77	70/4580 (1.5%)
1	E	2.14	110/3373 (3.3%)	1.69	59/4580 (1.3%)
1	F	2.25	118/3373 (3.5%)	1.87	76/4580 (1.7%)
1	G	2.13	104/3373 (3.1%)	1.71	59/4580 (1.3%)
1	H	2.13	97/3373 (2.9%)	1.80	79/4580 (1.7%)
1	I	2.20	114/3373 (3.4%)	1.80	81/4580 (1.8%)
1	J	2.24	135/3373 (4.0%)	1.79	77/4580 (1.7%)
1	K	2.16	106/3373 (3.1%)	1.72	63/4580 (1.4%)
1	L	2.19	105/3373 (3.1%)	1.68	57/4580 (1.2%)
1	M	2.24	134/3373 (4.0%)	1.70	57/4580 (1.2%)
1	N	2.15	106/3373 (3.1%)	1.70	56/4580 (1.2%)
1	O	2.20	104/3373 (3.1%)	1.70	62/4580 (1.4%)
All	All	2.19	1681/50595 (3.3%)	1.75	1014/68700 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	D	0	1
1	F	0	1
1	I	0	3
1	J	0	1
1	O	0	1
All	All	0	12

The worst 5 of 1681 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	467	LYS	CD-CE	15.78	1.90	1.51
1	N	152	LYS	CE-NZ	15.76	1.88	1.49
1	M	152	LYS	CE-NZ	15.45	1.87	1.49
1	A	26	GLU	CD-OE1	14.40	1.41	1.25
1	A	391	SER	CB-OG	14.30	1.60	1.42

The worst 5 of 1014 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	336	ARG	NE-CZ-NH2	-20.83	109.88	120.30
1	F	336	ARG	NE-CZ-NH2	-17.28	111.66	120.30
1	C	109	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	C	251	ARG	NE-CZ-NH1	16.29	128.44	120.30
1	L	30	ARG	NE-CZ-NH1	-16.14	112.23	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	PHE	Sidechain
1	A	35	TYR	Sidechain
1	A	468	PHE	Sidechain
1	B	231	TYR	Sidechain
1	B	462	PHE	Sidechain

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	3290	0	3191	235	0
1	B	3290	0	3191	243	0
1	C	3290	0	3191	282	0
1	D	3290	0	3191	251	0
1	E	3290	0	3191	251	0
1	F	3290	0	3191	283	0
1	G	3290	0	3191	222	0
1	H	3290	0	3191	219	0
1	I	3290	0	3191	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3290	0	3191	221	0
1	K	3290	0	3191	249	0
1	L	3290	0	3191	286	0
1	M	3290	0	3191	279	0
1	N	3290	0	3191	245	0
1	O	3290	0	3191	260	0
All	All	49350	0	47865	3403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 3403 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:K:379:ILE:CG1	1:K:379:ILE:CD1	1.74	1.65
1:F:117:ILE:CG1	1:F:117:ILE:CD1	1.75	1.65
1:G:254:GLN:CB	1:G:254:GLN:CG	1.75	1.63
1:N:76:LYS:CD	1:N:76:LYS:CG	1.75	1.62
1:O:228:ILE:CD1	1:O:228:ILE:CG1	1.76	1.62

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	413/423 (98%)	348 (84%)	52 (13%)	13 (3%)	4 23
1	B	413/423 (98%)	343 (83%)	55 (13%)	15 (4%)	3 20
1	C	413/423 (98%)	344 (83%)	47 (11%)	22 (5%)	2 12
1	D	413/423 (98%)	352 (85%)	50 (12%)	11 (3%)	5 26
1	E	413/423 (98%)	336 (81%)	64 (16%)	13 (3%)	4 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	413/423 (98%)	346 (84%)	55 (13%)	12 (3%)	4	24
1	G	413/423 (98%)	353 (86%)	46 (11%)	14 (3%)	3	22
1	H	413/423 (98%)	347 (84%)	50 (12%)	16 (4%)	3	18
1	I	413/423 (98%)	343 (83%)	53 (13%)	17 (4%)	3	17
1	J	413/423 (98%)	351 (85%)	48 (12%)	14 (3%)	3	22
1	K	413/423 (98%)	349 (84%)	49 (12%)	15 (4%)	3	20
1	L	413/423 (98%)	348 (84%)	52 (13%)	13 (3%)	4	23
1	M	413/423 (98%)	338 (82%)	60 (14%)	15 (4%)	3	20
1	N	413/423 (98%)	345 (84%)	56 (14%)	12 (3%)	4	24
1	O	413/423 (98%)	335 (81%)	59 (14%)	19 (5%)	2	15
All	All	6195/6345 (98%)	5178 (84%)	796 (13%)	221 (4%)	3	20

5 of 221 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	LEU
1	A	126	LEU
1	A	337	SER
1	B	177	ALA
1	B	323	TRP

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	367/369 (100%)	332 (90%)	35 (10%)	8	29
1	B	367/369 (100%)	318 (87%)	49 (13%)	4	16
1	C	367/369 (100%)	324 (88%)	43 (12%)	5	21
1	D	367/369 (100%)	330 (90%)	37 (10%)	7	27
1	E	367/369 (100%)	329 (90%)	38 (10%)	7	25
1	F	367/369 (100%)	322 (88%)	45 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	367/369 (100%)	328 (89%)	39 (11%)	6	25
1	H	367/369 (100%)	323 (88%)	44 (12%)	5	20
1	I	367/369 (100%)	323 (88%)	44 (12%)	5	20
1	J	367/369 (100%)	326 (89%)	41 (11%)	6	23
1	K	367/369 (100%)	327 (89%)	40 (11%)	6	24
1	L	367/369 (100%)	324 (88%)	43 (12%)	5	21
1	M	367/369 (100%)	334 (91%)	33 (9%)	9	32
1	N	367/369 (100%)	322 (88%)	45 (12%)	4	20
1	O	367/369 (100%)	325 (89%)	42 (11%)	5	22
All	All	5505/5535 (100%)	4887 (89%)	618 (11%)	6	23

5 of 618 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	118	SER
1	N	393	ASN
1	L	225	CYS
1	L	117	ILE
1	M	257	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	133	ASN
1	L	133	ASN
1	J	192	ASN
1	K	133	ASN
1	L	339	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 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 (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	417/423 (98%)	-0.03	7 (1%)	70	68	21, 52, 109, 134	0
1	B	417/423 (98%)	-0.01	9 (2%)	62	60	25, 51, 110, 139	0
1	C	417/423 (98%)	0.08	12 (2%)	51	50	22, 56, 109, 138	0
1	D	417/423 (98%)	0.08	19 (4%)	32	30	24, 56, 110, 146	0
1	E	417/423 (98%)	0.06	13 (3%)	49	48	24, 54, 112, 139	0
1	F	417/423 (98%)	0.03	23 (5%)	25	23	20, 51, 111, 140	0
1	G	417/423 (98%)	-0.02	9 (2%)	62	60	22, 55, 107, 133	0
1	H	417/423 (98%)	0.19	16 (3%)	40	37	21, 57, 112, 140	0
1	I	417/423 (98%)	0.09	13 (3%)	49	48	22, 56, 110, 140	0
1	J	417/423 (98%)	0.02	11 (2%)	56	53	21, 53, 111, 141	0
1	K	417/423 (98%)	0.23	20 (4%)	30	28	25, 66, 112, 140	0
1	L	417/423 (98%)	0.19	13 (3%)	49	48	26, 60, 111, 145	0
1	M	417/423 (98%)	0.22	19 (4%)	32	30	27, 63, 116, 141	0
1	N	417/423 (98%)	0.17	12 (2%)	51	50	22, 62, 113, 144	0
1	O	417/423 (98%)	0.27	25 (5%)	21	21	24, 61, 112, 143	0
All	All	6255/6345 (98%)	0.11	221 (3%)	44	42	20, 57, 111, 146	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	178	ASN	12.6
1	H	176	ASN	11.0
1	O	176	ASN	10.2
1	L	178	ASN	9.8
1	I	178	ASN	9.5

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

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

6.3 Carbohydrates (i)

There are no 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.