



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:05 PM GMT

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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

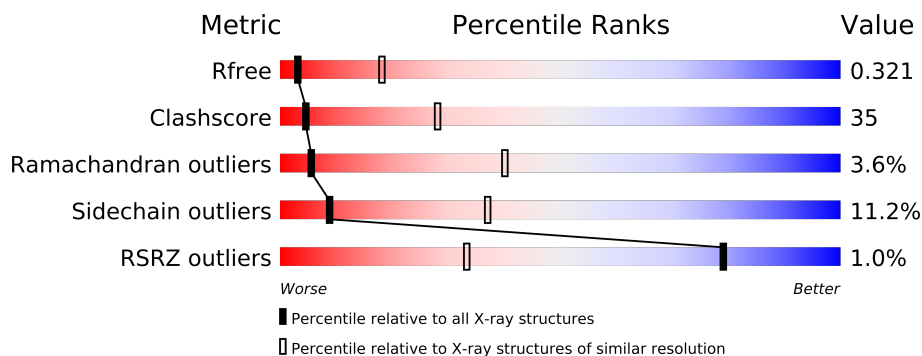
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	423	
1	B	423	
1	C	423	
1	D	423	
1	E	423	
1	F	423	
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	
1	M	423	
1	N	423	

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Mol	Chain	Length	Quality of chain
1	O	423	 A horizontal bar chart representing the quality of the protein chain. The bar is divided into segments of different colors: green, yellow, orange, and red, indicating different levels of quality or validation scores.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 49350 atoms, of which 0 are hydrogen and 0 are deuterium.

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	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	B	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	C	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	D	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	E	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	F	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	G	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	H	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	I	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	J	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	K	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	L	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	M	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	N	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	O	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			

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	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	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	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	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	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	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	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	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	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	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	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	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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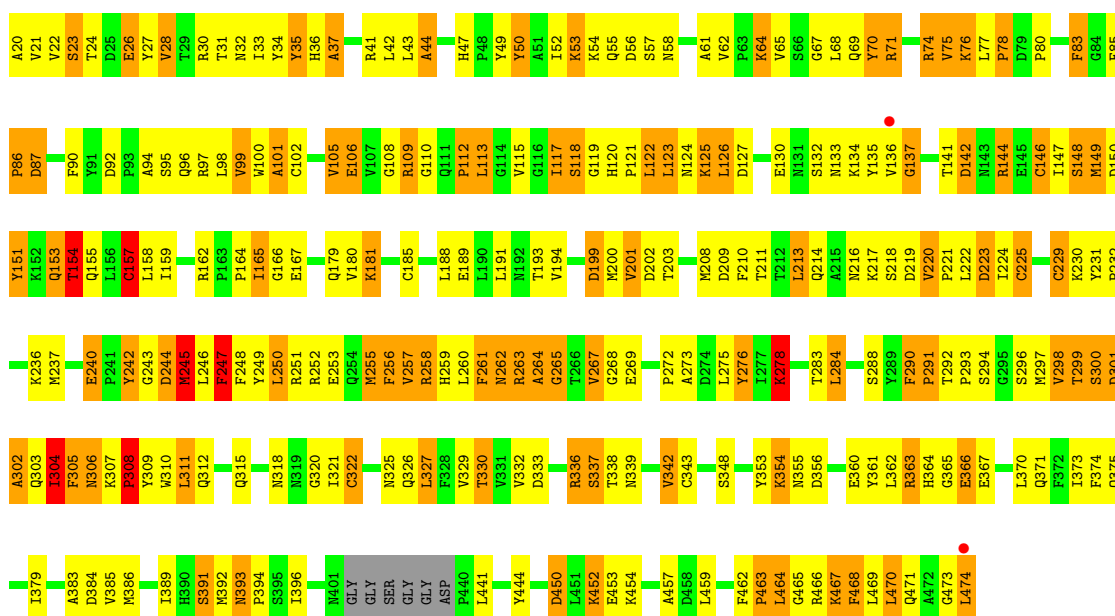
Chain	Residue	Modelled	Actual	Comment	Reference
M	175	SER	CYS	ENGINEERED	UNP P27232
M	402	GLY	-	LINKER	UNP P27232
M	403	GLY	-	LINKER	UNP P27232
M	404	SER	-	LINKER	UNP P27232
M	405	GLY	-	LINKER	UNP P27232
M	406	GLY	-	LINKER	UNP P27232
N	20	ALA	-	EXPRESSION TAG	UNP P27232
N	175	SER	CYS	ENGINEERED	UNP P27232
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	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

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

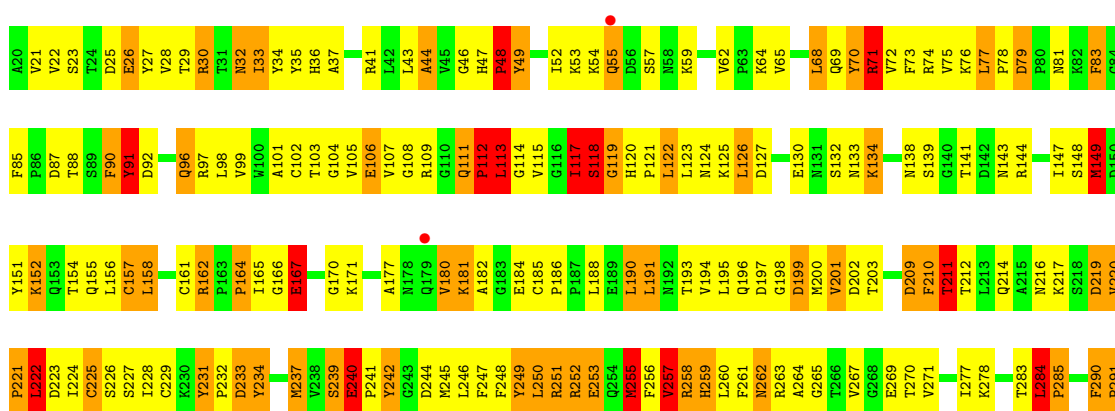
• Molecule 1: Major capsid protein L1

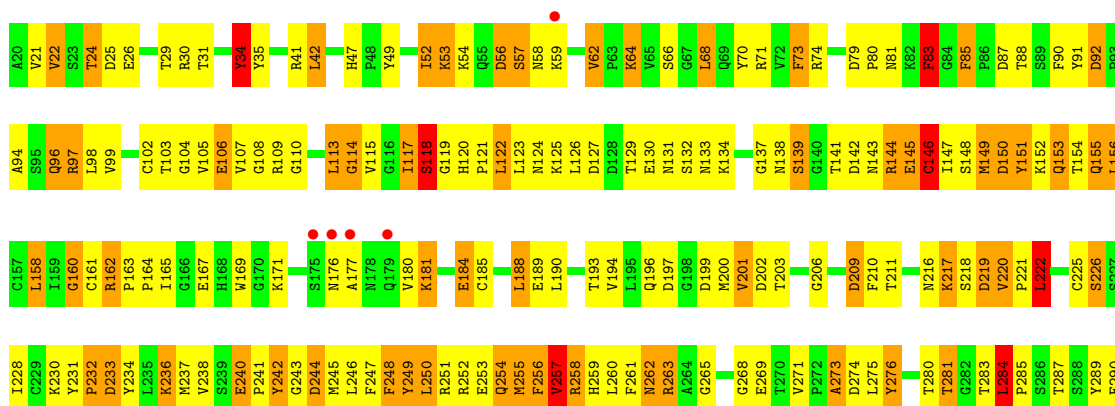
Chain A:

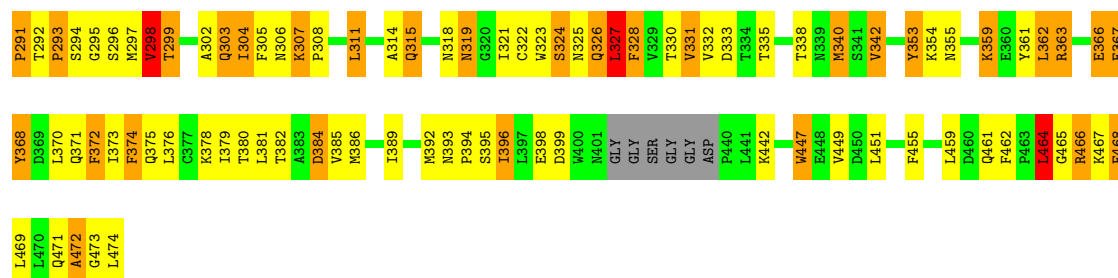


• Molecule 1: Major capsid protein L1

Chain B:

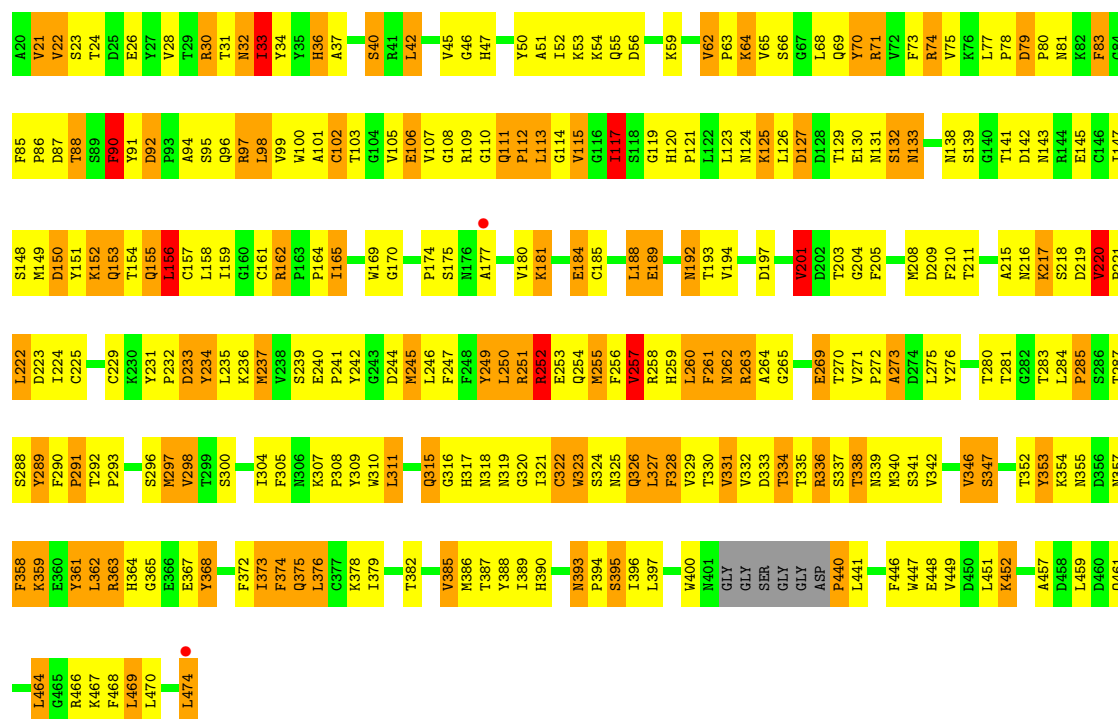






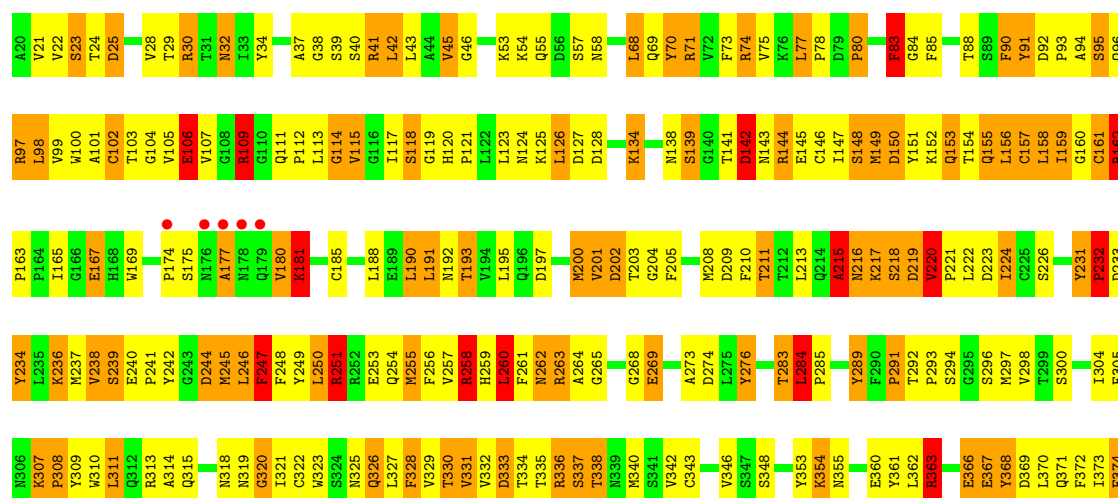
• Molecule 1: Major capsid protein L1

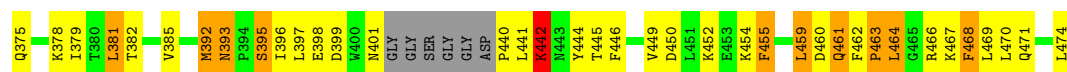
Chain E:



• Molecule 1: Major capsid protein L1

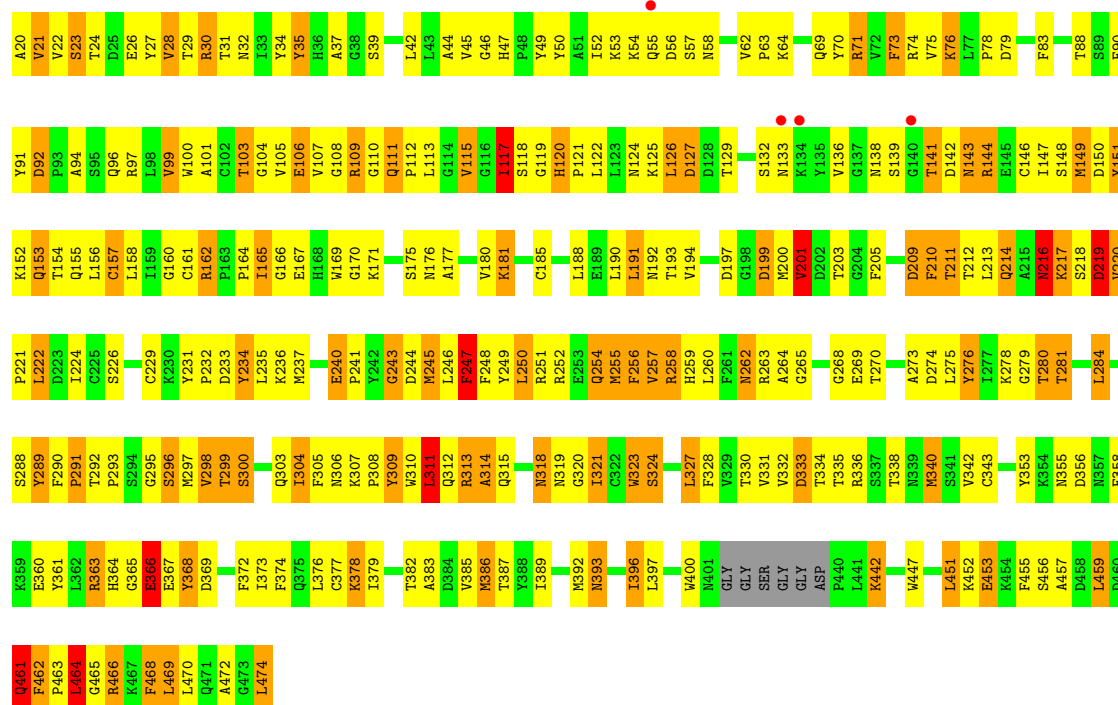
Chain F:





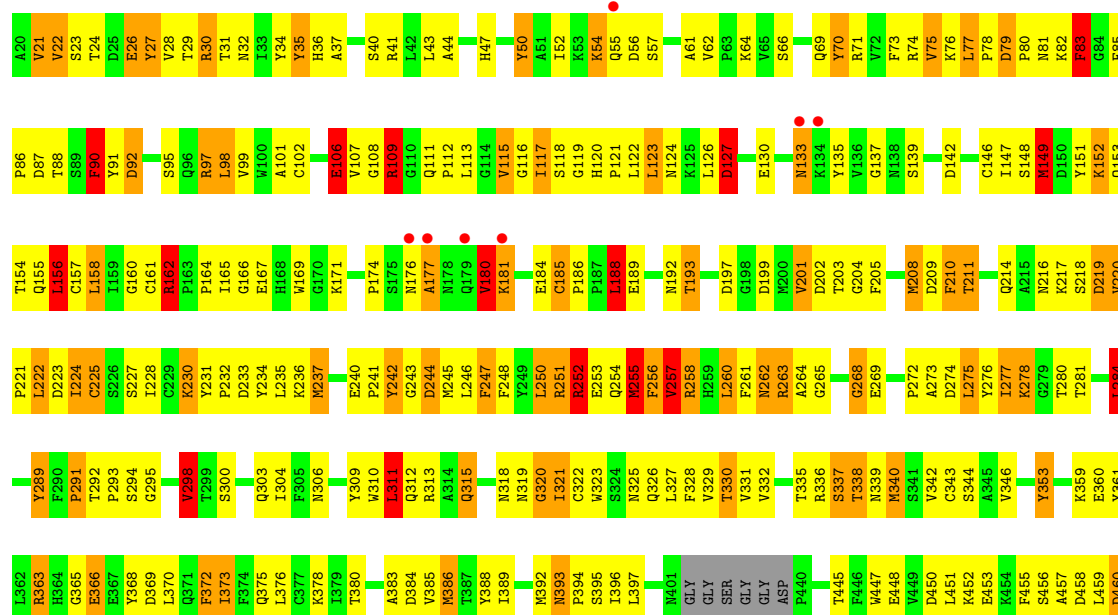
Molecule 1: Major capsid protein L1

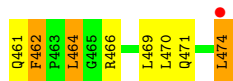
Chain G:



Molecule 1: Major capsid protein L1

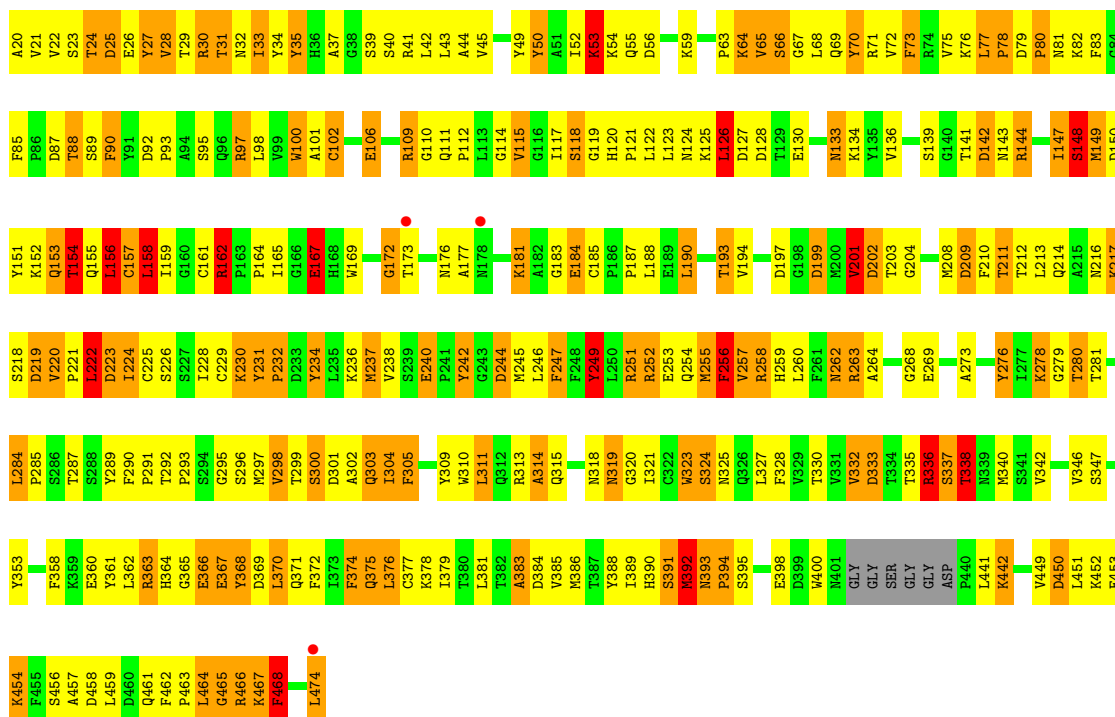
Chain H:





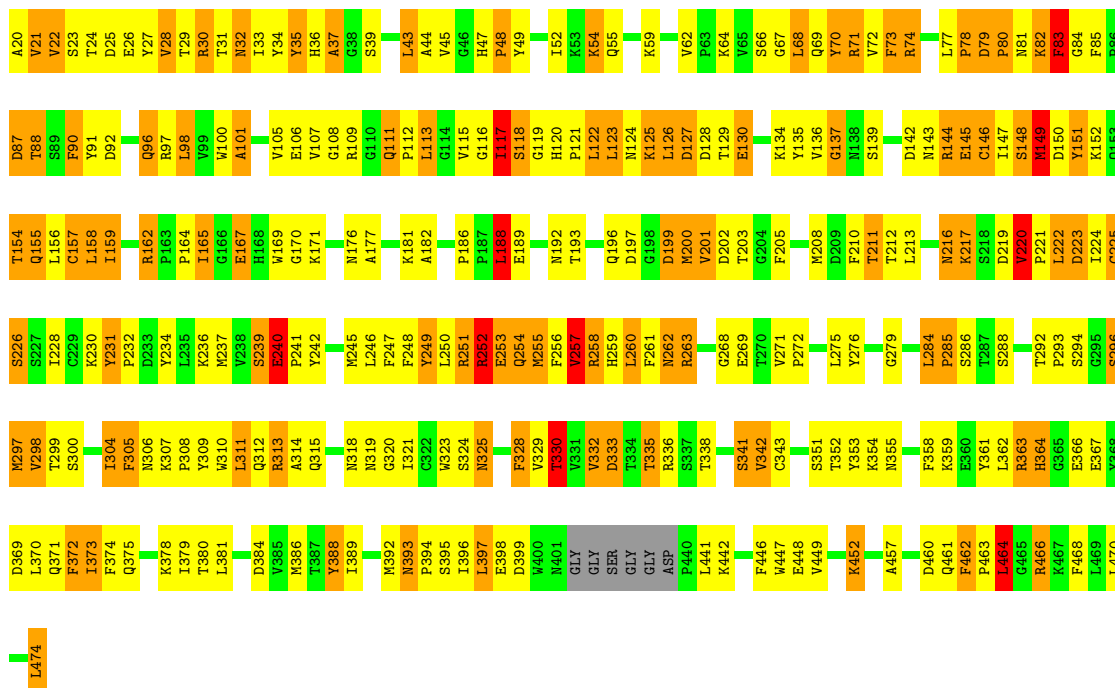
● Molecule 1: Major capsid protein L1

Chain I:



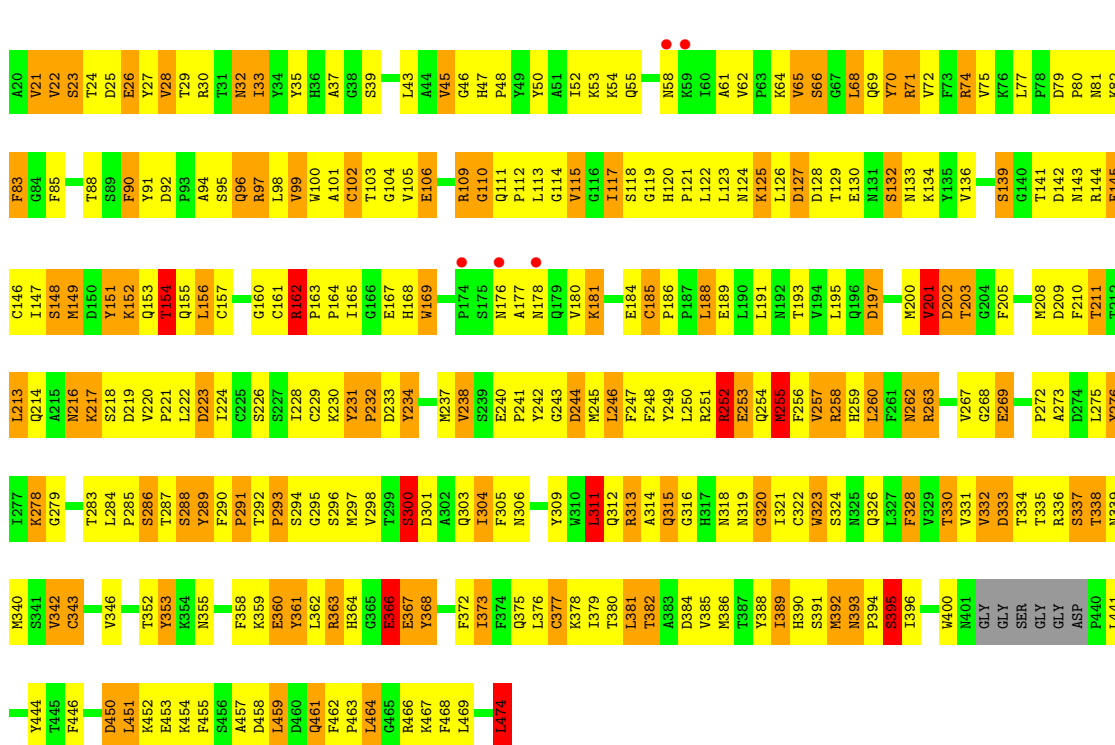
● Molecule 1: Major capsid protein L1

Chain J:



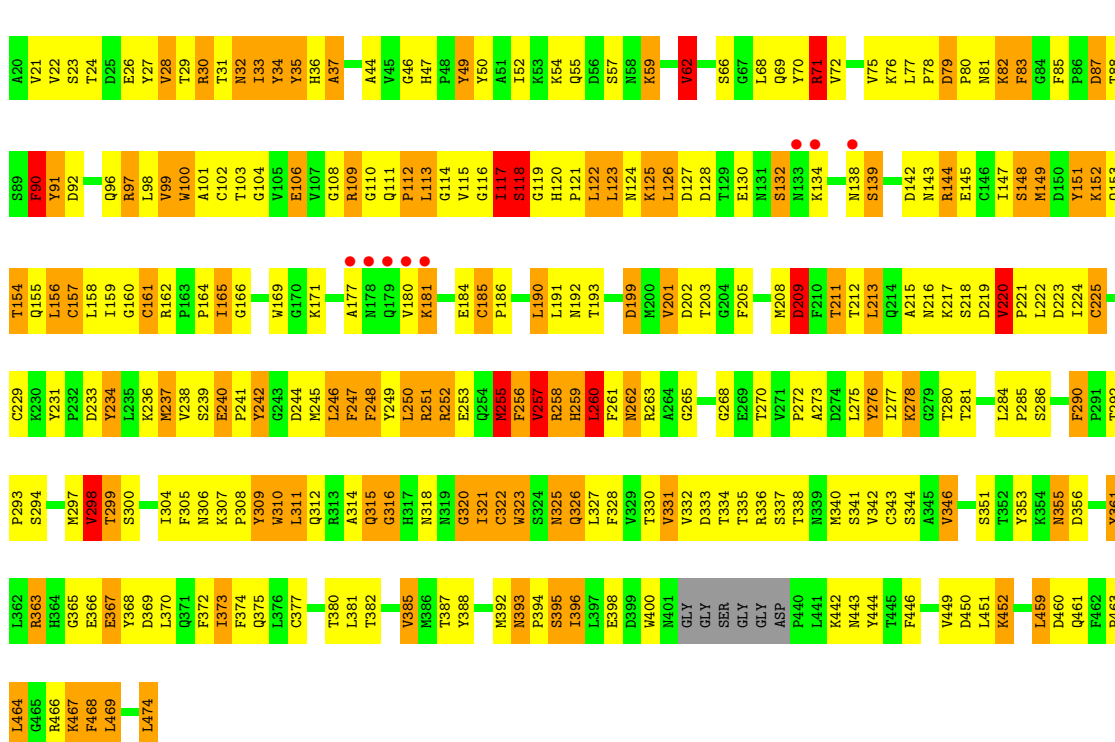
- Molecule 1: Major capsid protein L1

Chain K:



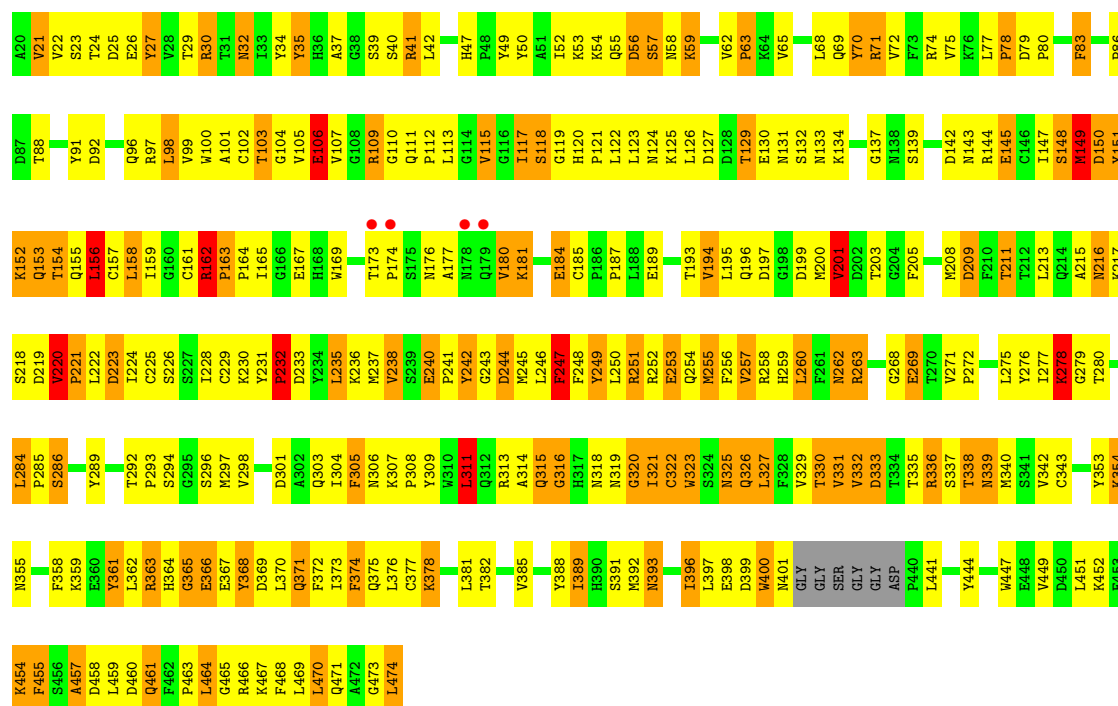
- Molecule 1: Major capsid protein L1

Chain L:



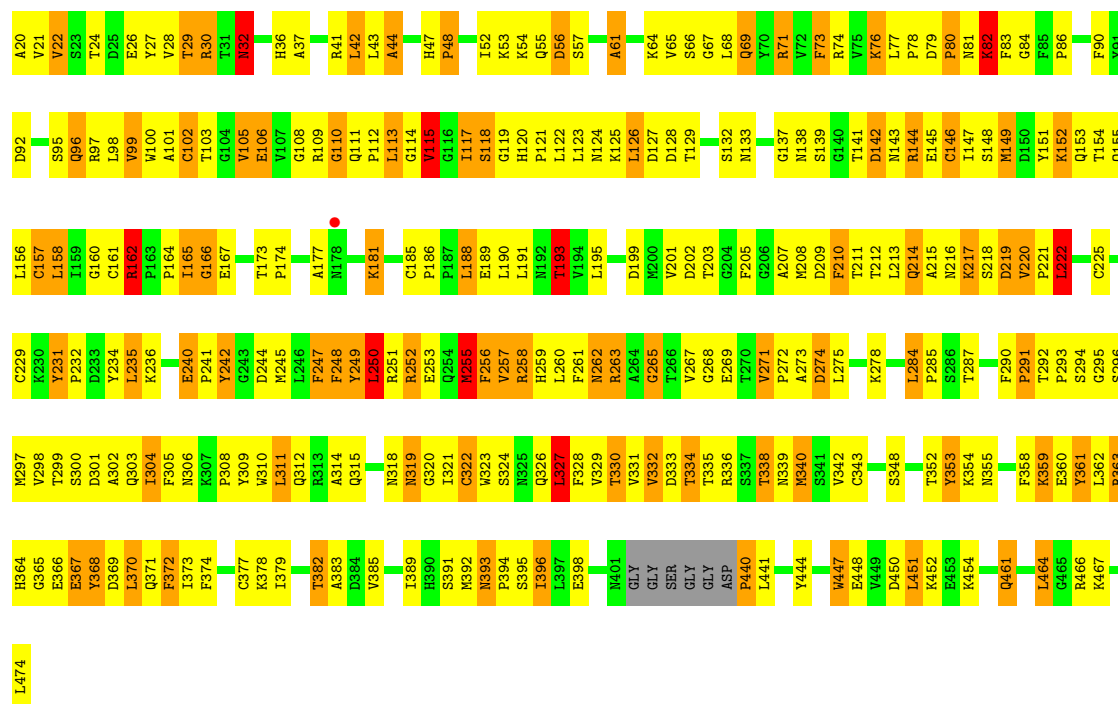
- Molecule 1: Major capsid protein L1

Chain M:



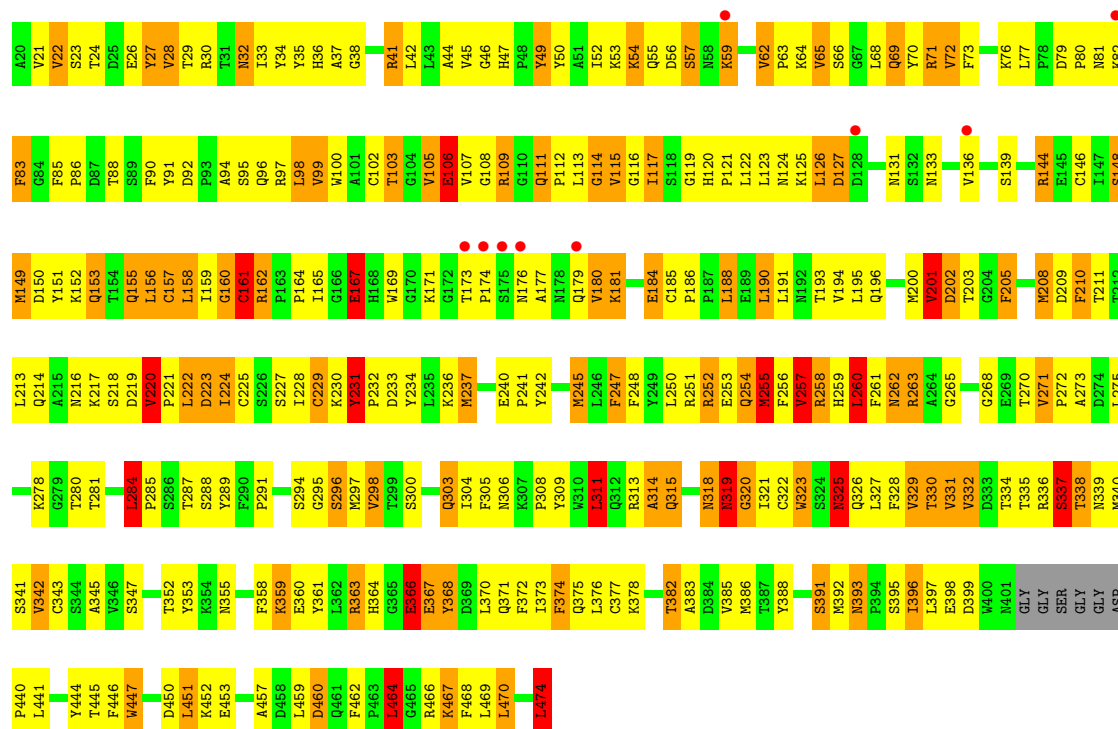
- Molecule 1: Major capsid protein L1

Chain N:



- Molecule 1: Major capsid protein L1

Chain O:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.315 , 0.348 0.302 , 0.321	Depositor DCC
R_{free} test set	7364 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 7.8	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 146166 reflections	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.*

¹Intensities estimated from amplitudes.

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	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(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3290	0	3191	219	0
1	I	3290	0	3191	252	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

The worst 5 of 3403 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:379:ILE:CG1	1:K:379:ILE:CD1	1.74	1.65
1:F:117:ILE:CD1	1:F:117:ILE:CG1	1.75	1.65
1:G:254:GLN:CB	1:G:254:GLN:CG	1.75	1.63
1:O:228:ILE:CD1	1:O:228:ILE:CG1	1.76	1.62
1:N:76:LYS:CG	1:N:76:LYS:CD	1.75	1.62

There are no symmetry-related clashes.

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	413/423 (98%)	348 (84%)	52 (13%)	13 (3%)	7	45
1	B	413/423 (98%)	343 (83%)	55 (13%)	15 (4%)	5	40
1	C	413/423 (98%)	344 (83%)	47 (11%)	22 (5%)	3	26
1	D	413/423 (98%)	352 (85%)	50 (12%)	11 (3%)	8	49
1	E	413/423 (98%)	336 (81%)	64 (16%)	13 (3%)	7	45
1	F	413/423 (98%)	346 (84%)	55 (13%)	12 (3%)	7	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	413/423 (98%)	353 (86%)	46 (11%)	14 (3%)	6	42
1	H	413/423 (98%)	347 (84%)	50 (12%)	16 (4%)	5	37
1	I	413/423 (98%)	343 (83%)	53 (13%)	17 (4%)	4	35
1	J	413/423 (98%)	351 (85%)	48 (12%)	14 (3%)	6	42
1	K	413/423 (98%)	349 (84%)	49 (12%)	15 (4%)	5	40
1	L	413/423 (98%)	348 (84%)	52 (13%)	13 (3%)	7	45
1	M	413/423 (98%)	338 (82%)	60 (14%)	15 (4%)	5	40
1	N	413/423 (98%)	345 (84%)	56 (14%)	12 (3%)	7	47
1	O	413/423 (98%)	335 (81%)	59 (14%)	19 (5%)	4	31
All	All	6195/6345 (98%)	5178 (84%)	796 (13%)	221 (4%)	5	40

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 ⓘ

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%)	12	46
1	B	367/369 (100%)	318 (87%)	49 (13%)	6	27
1	C	367/369 (100%)	324 (88%)	43 (12%)	8	35
1	D	367/369 (100%)	330 (90%)	37 (10%)	11	42
1	E	367/369 (100%)	329 (90%)	38 (10%)	10	41
1	F	367/369 (100%)	322 (88%)	45 (12%)	7	32
1	G	367/369 (100%)	328 (89%)	39 (11%)	10	40
1	H	367/369 (100%)	323 (88%)	44 (12%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	367/369 (100%)	323 (88%)	44 (12%)	7	33
1	J	367/369 (100%)	326 (89%)	41 (11%)	9	37
1	K	367/369 (100%)	327 (89%)	40 (11%)	9	38
1	L	367/369 (100%)	324 (88%)	43 (12%)	8	35
1	M	367/369 (100%)	334 (91%)	33 (9%)	14	50
1	N	367/369 (100%)	322 (88%)	45 (12%)	7	32
1	O	367/369 (100%)	325 (89%)	42 (11%)	8	36
All	All	5505/5535 (100%)	4887 (89%)	618 (11%)	9	37

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

Mol	Chain	Res	Type
1	G	340	MET
1	I	162	ARG
1	N	352	THR
1	H	83	PHE
1	H	257	VAL

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

Mol	Chain	Res	Type
1	H	32	ASN
1	I	262	ASN
1	N	461	GLN
1	H	96	GLN
1	H	315	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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%)	-0.06	2 (0%)	88 51	21, 52, 109, 134	0
1	B	417/423 (98%)	-0.05	3 (0%)	84 42	25, 51, 110, 139	0
1	C	417/423 (98%)	-0.00	6 (1%)	72 25	22, 56, 109, 138	0
1	D	417/423 (98%)	0.00	5 (1%)	75 29	24, 56, 110, 146	0
1	E	417/423 (98%)	-0.01	2 (0%)	88 51	24, 54, 112, 139	0
1	F	417/423 (98%)	-0.03	5 (1%)	75 29	20, 51, 111, 140	0
1	G	417/423 (98%)	-0.05	4 (0%)	79 33	22, 55, 107, 133	0
1	H	417/423 (98%)	0.06	8 (1%)	64 20	21, 57, 112, 140	0
1	I	417/423 (98%)	0.01	3 (0%)	84 42	22, 56, 110, 140	0
1	J	417/423 (98%)	-0.03	0	100 100	21, 53, 111, 141	0
1	K	417/423 (98%)	0.08	5 (1%)	75 29	25, 66, 112, 140	0
1	L	417/423 (98%)	0.07	8 (1%)	64 20	26, 60, 111, 145	0
1	M	417/423 (98%)	0.09	4 (0%)	79 33	27, 63, 116, 141	0
1	N	417/423 (98%)	0.06	1 (0%)	93 70	22, 62, 113, 144	0
1	O	417/423 (98%)	0.11	9 (2%)	59 16	24, 61, 112, 143	0
All	All	6255/6345 (98%)	0.02	65 (1%)	79 33	20, 57, 111, 146	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	178	ASN	5.7
1	H	176	ASN	5.2
1	M	179	GLN	4.9
1	D	179	GLN	4.8
1	O	176	ASN	4.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.