



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:07 PM UTC

PDB ID : 3SHM / pdb_00003shm
Title : Structure-function Analysis of Receptor Binding in Adeno-Associated Virus Serotype 6 (AAV-6)
Authors : Xie, Q.; Lerch, T.F.; Meyer, N.L.; Chapman, M.S.
Deposited on : 2011-06-16
Resolution : 3.02 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 ⓘ 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

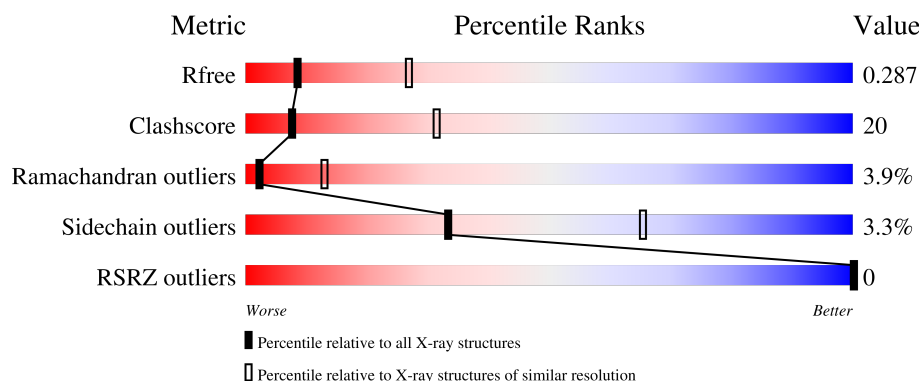
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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.



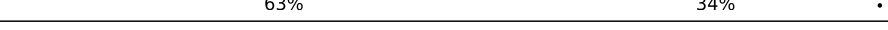
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	516	 63% 34% .
1	B	516	 61% 35% .
1	C	516	 63% 33% .
1	D	516	 60% 36% .
1	E	516	 61% 35% .

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Mol	Chain	Length	Quality of chain
1	F	516	 57% 39% .
1	G	516	 60% 37% .
1	H	516	 58% 38% .
1	I	516	 58% 39% .
1	J	516	 58% 39% .
1	K	516	 60% 36% .
1	L	516	 61% 36% .
1	M	516	 63% 34% .
1	N	516	 59% 38% .
1	O	516	 60% 37% .
1	P	516	 58% 38% .
1	Q	516	 59% 38% .
1	R	516	 58% 38% .
1	S	516	 63% 34% .
1	T	516	 60% 36% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 82000 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	B	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	C	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	D	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	E	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	F	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	G	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	H	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	I	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	J	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	K	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	L	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	M	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	N	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	O	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	P	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			

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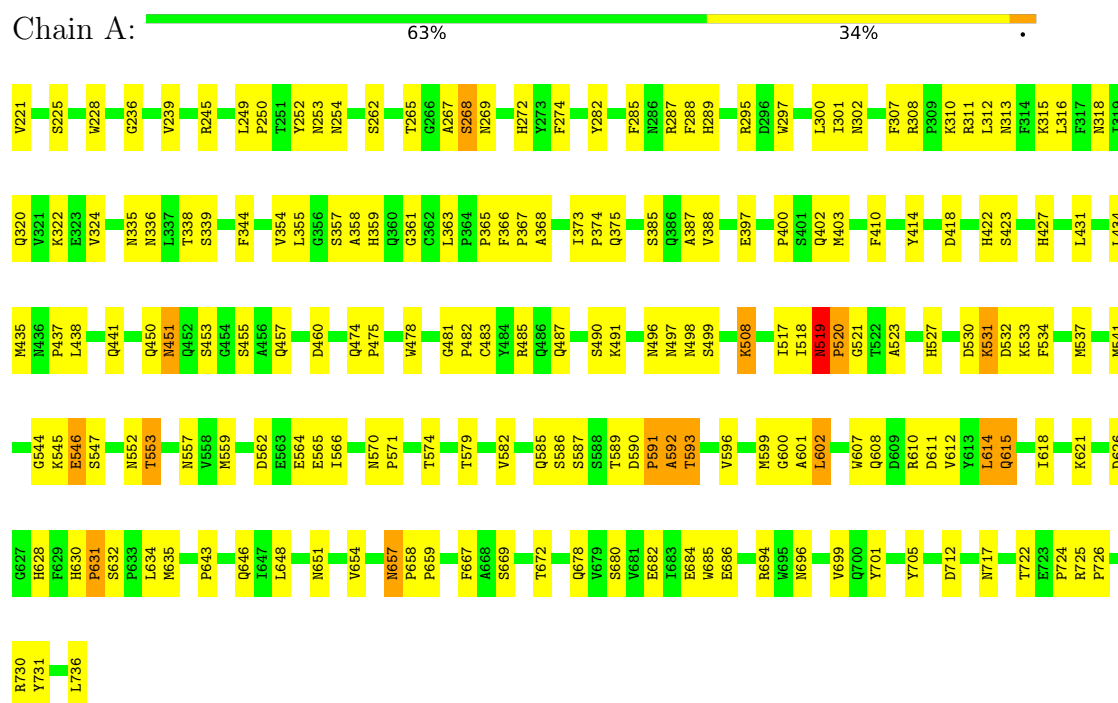
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0
1	R	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0
1	S	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0
1	T	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0

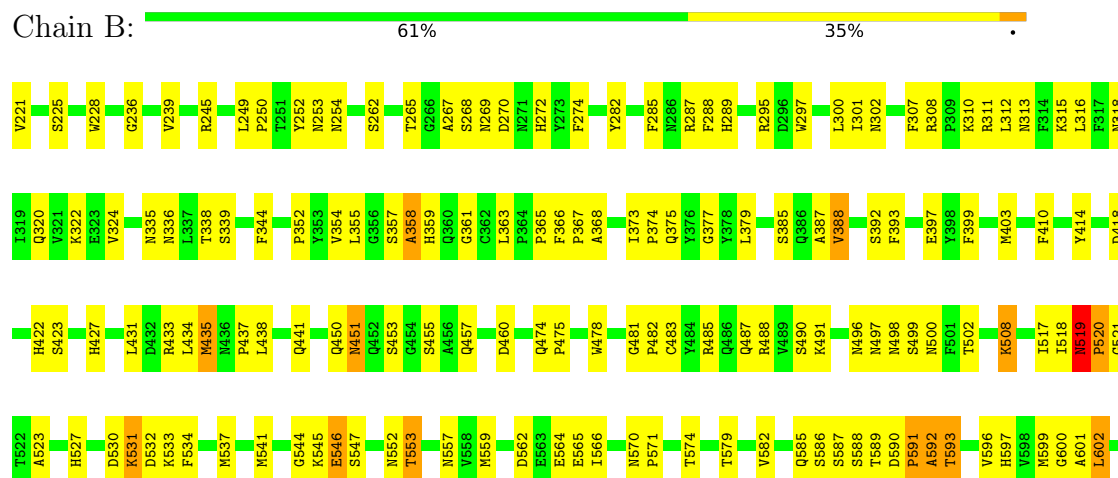
3 Residue-property plots

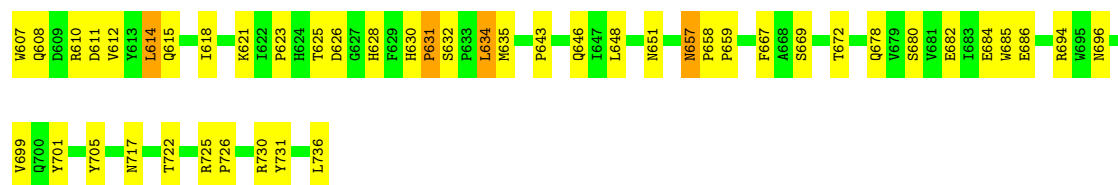
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Capsid protein VP1



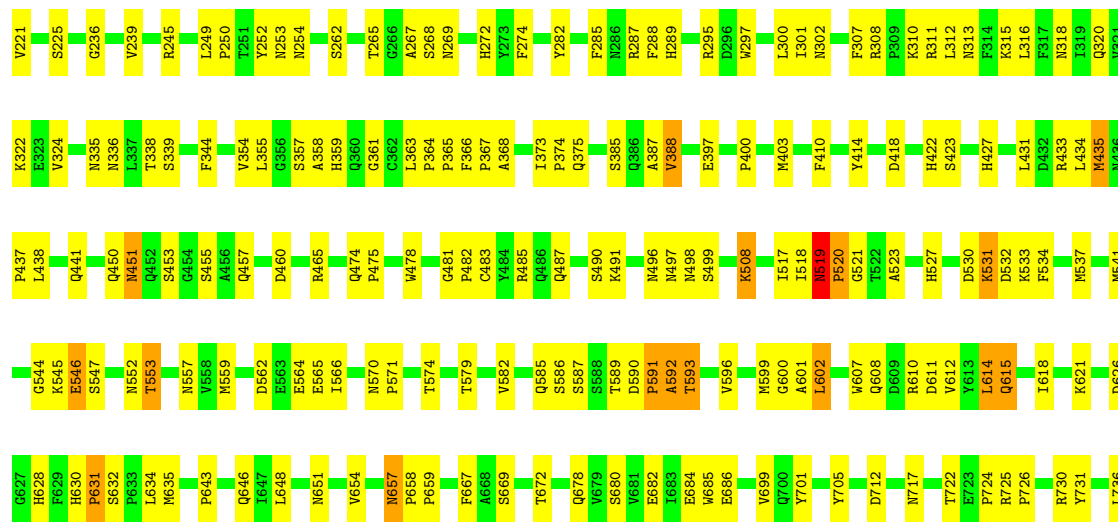
• Molecule 1: Capsid protein VP1





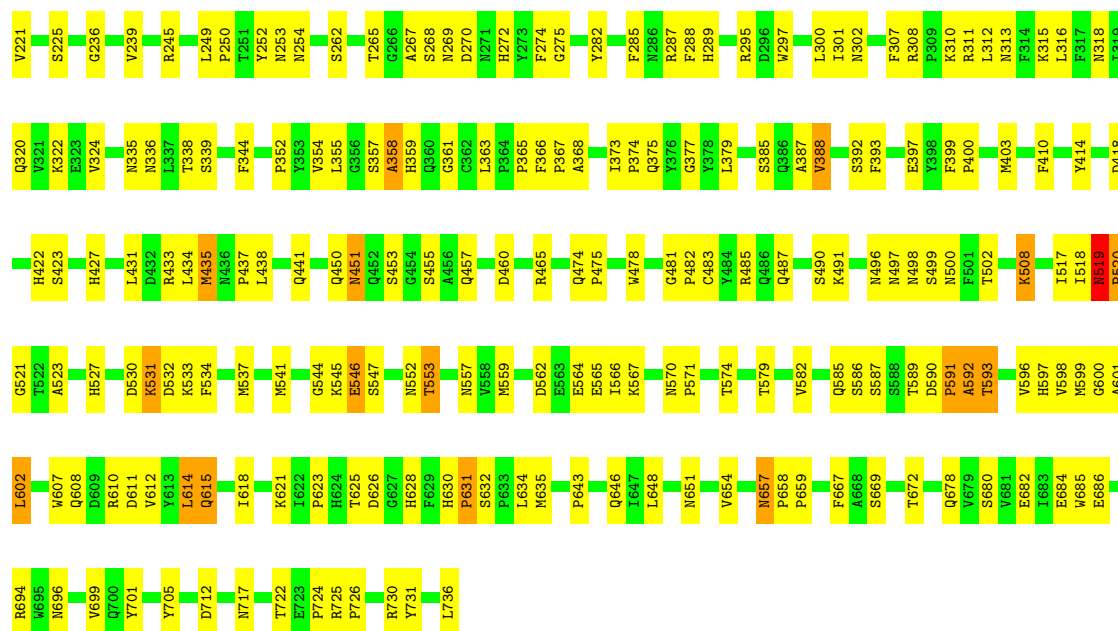
• Molecule 1: Capsid protein VP1

Chain C: 63% 33%



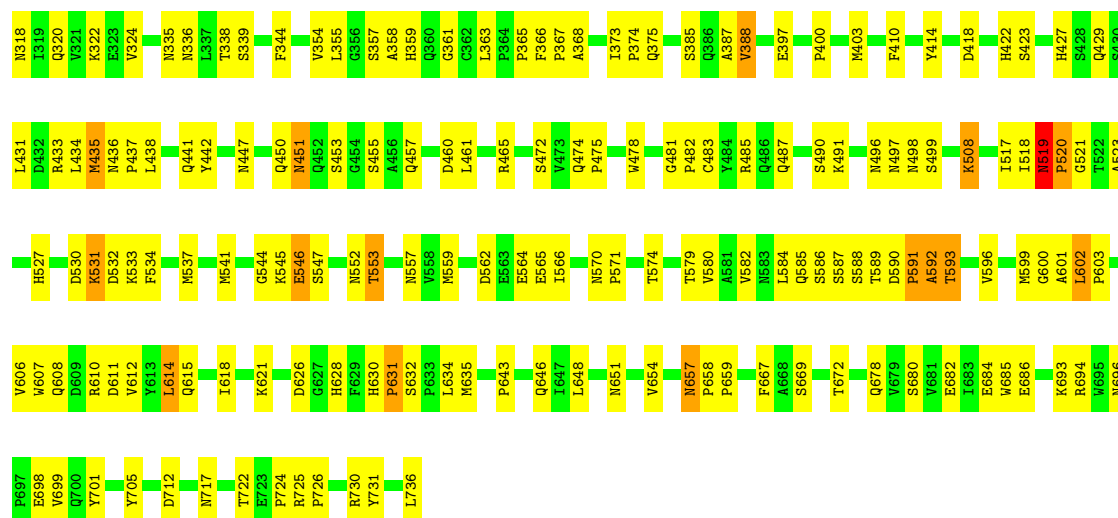
• Molecule 1: Capsid protein VP1

Chain D: 60% 36%



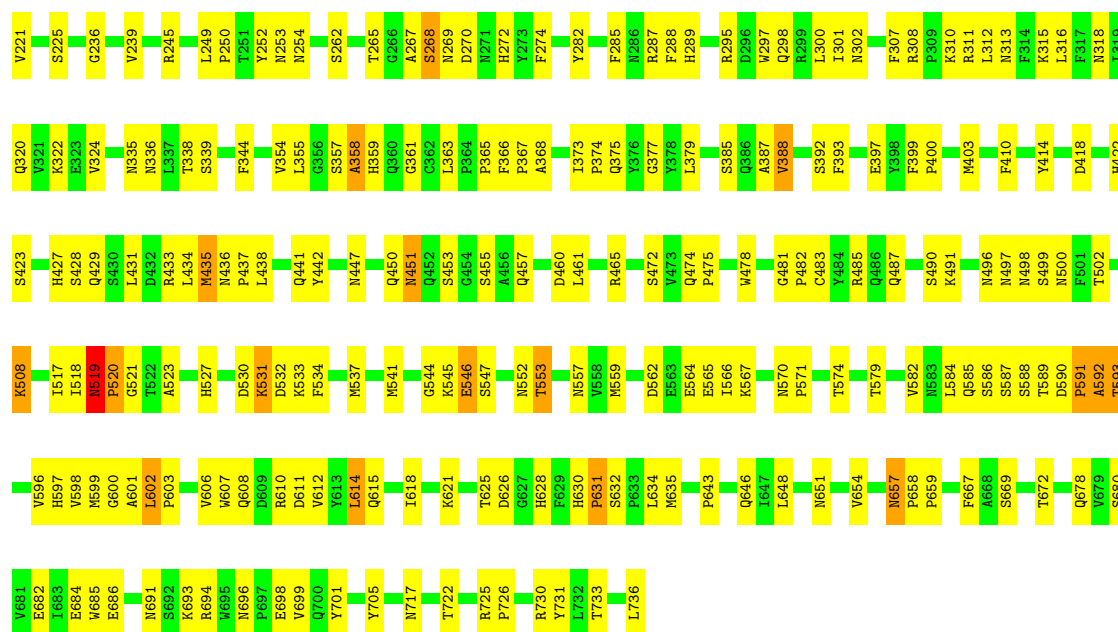
• Molecule 1: Capsid protein VP1





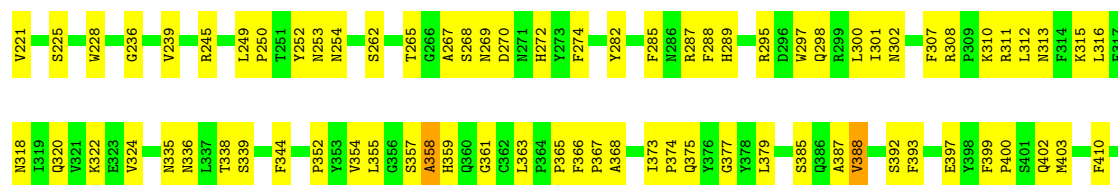
• Molecule 1: Capsid protein VP1

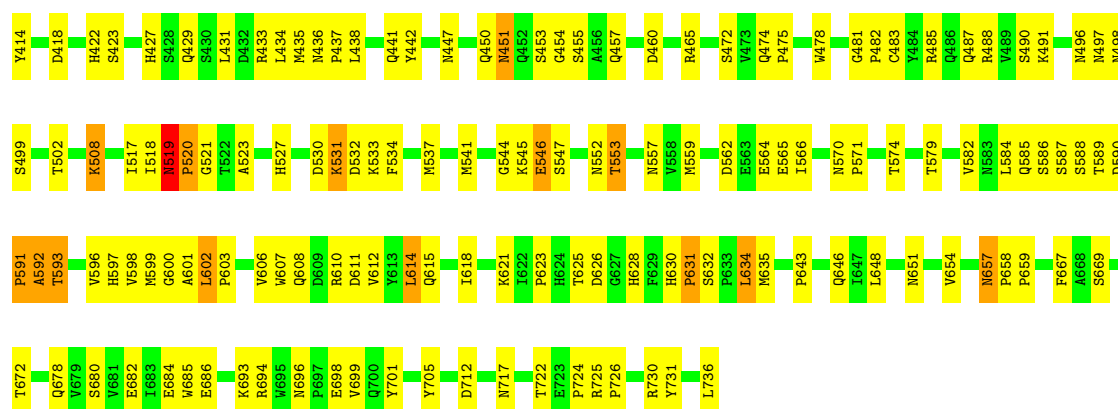
Chain H: 58% 38%



• Molecule 1: Capsid protein VP1

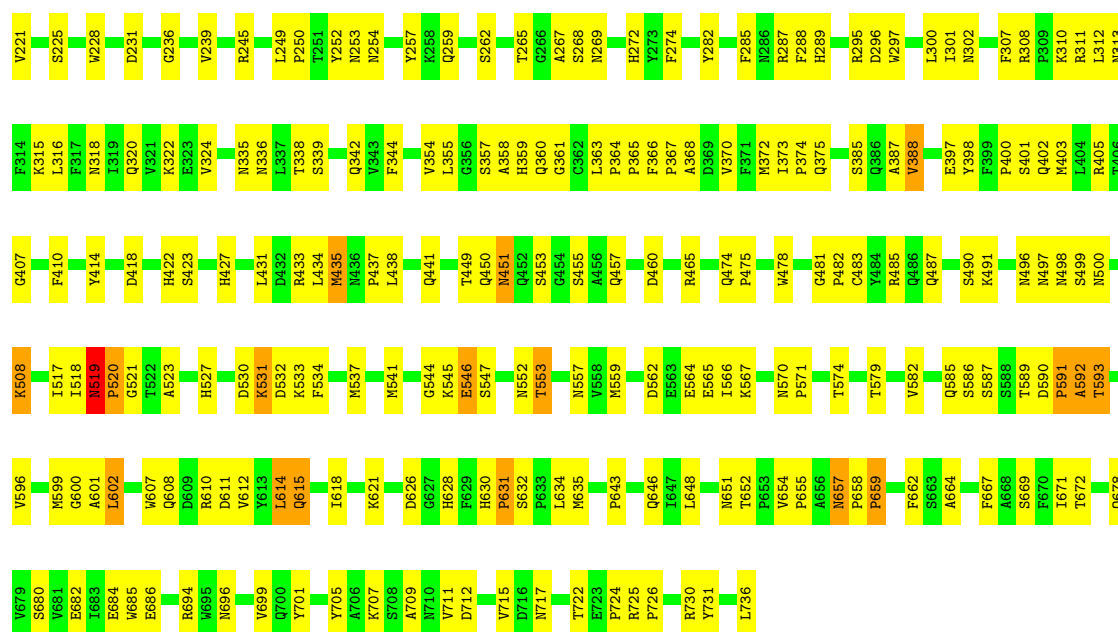
Chain I: 58% 39%





• Molecule 1: Capsid protein VP1

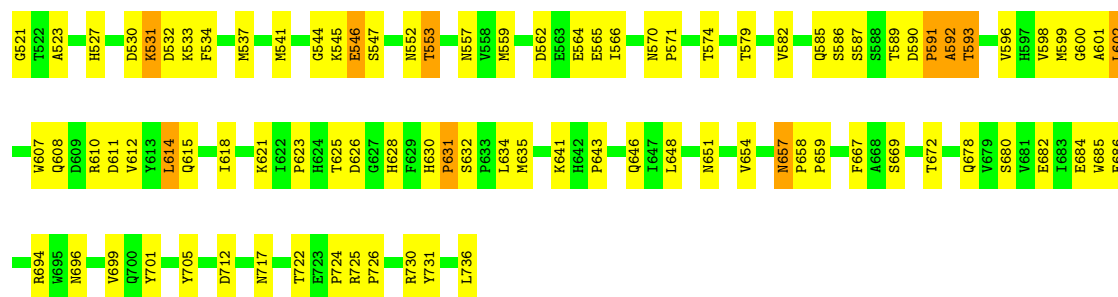
Chain J: 58% 39% •



• Molecule 1: Capsid protein VP1

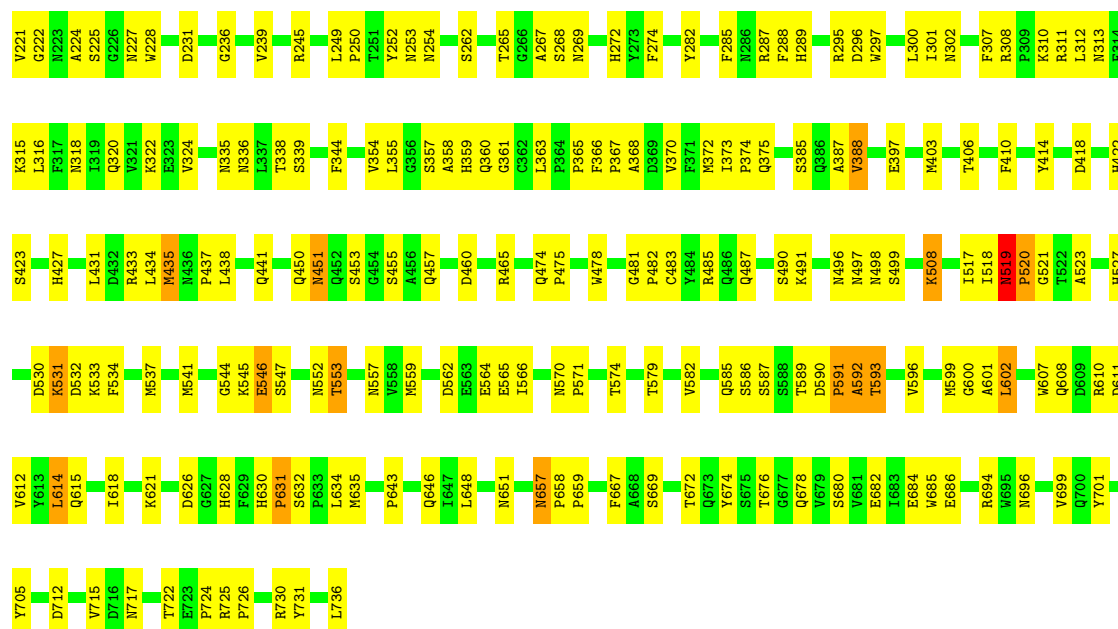
Chain K: 60% 36% •





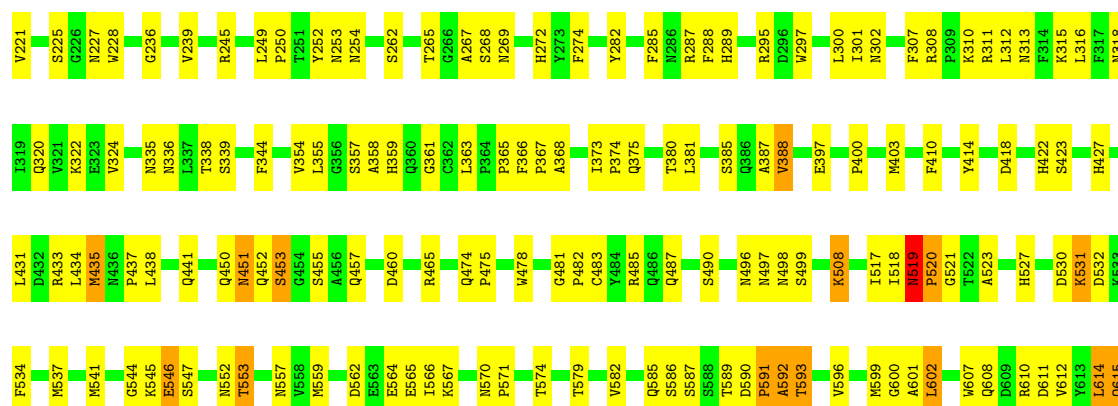
• Molecule 1: Capsid protein VP1

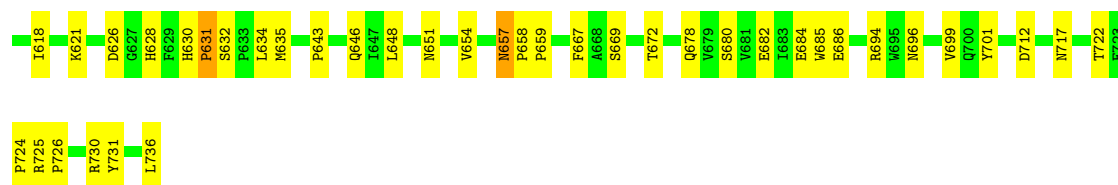
Chain L: 61% 36%



• Molecule 1: Capsid protein VP1

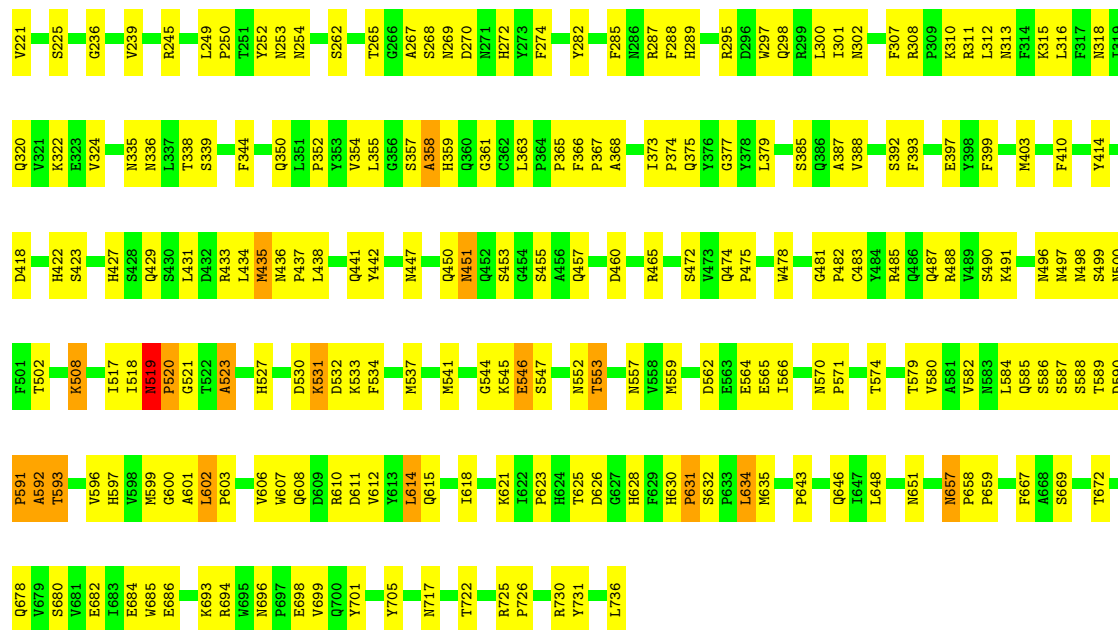
Chain M: 63% 34%





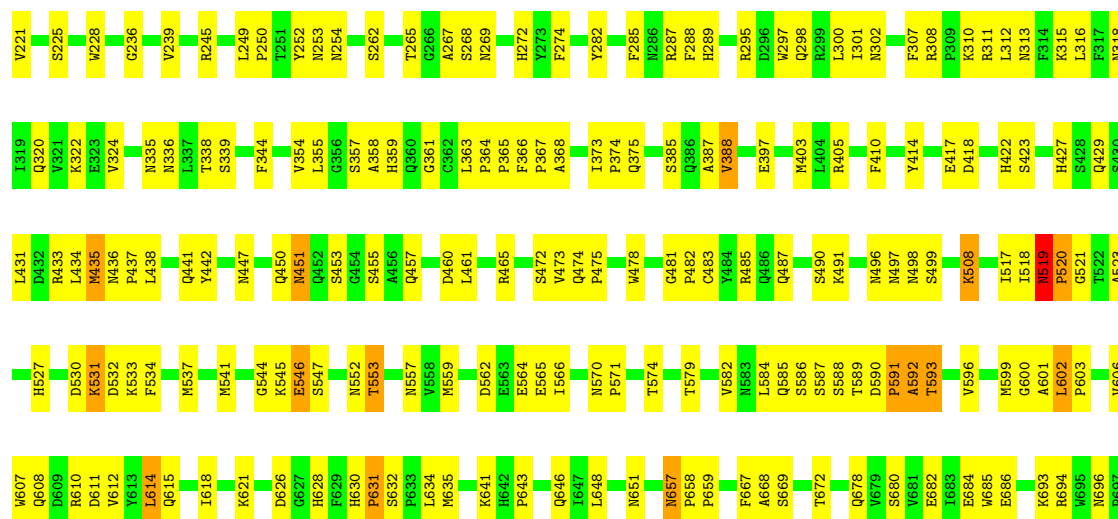
• Molecule 1: Capsid protein VP1

Chain N: 59% 38%



• Molecule 1: Capsid protein VP1

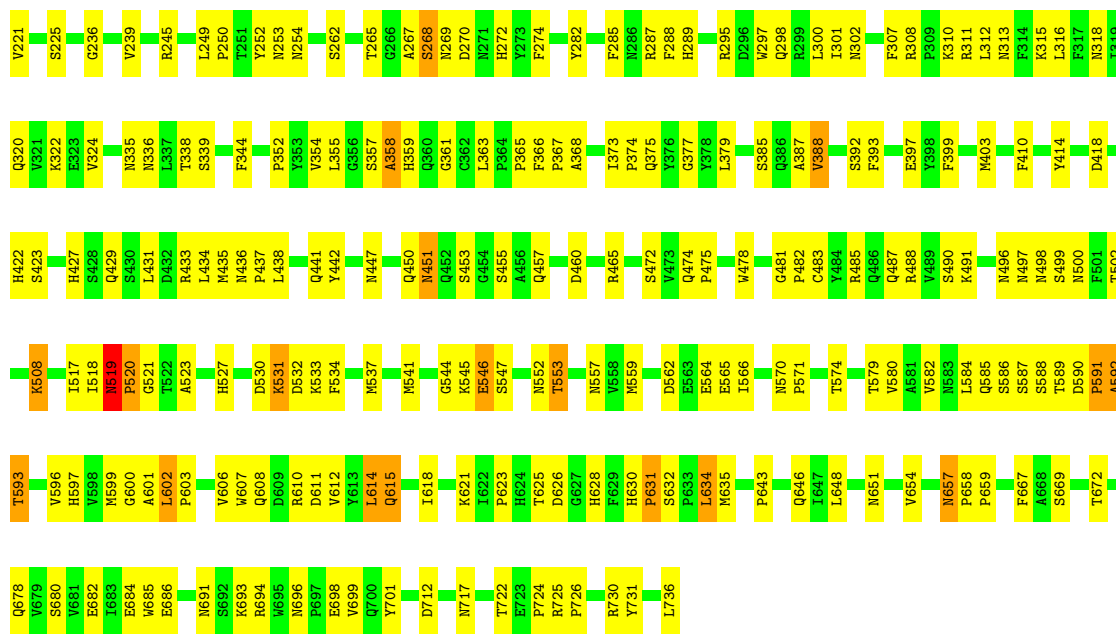
Chain O: 60% 37%





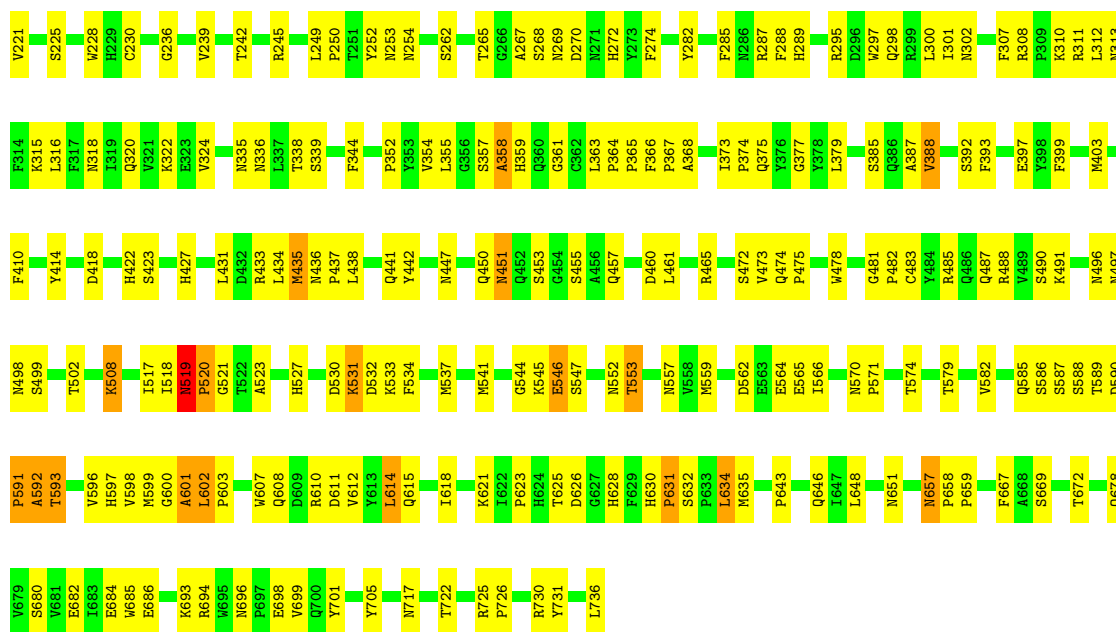
• Molecule 1: Capsid protein VP1

Chain P:  58% 38%



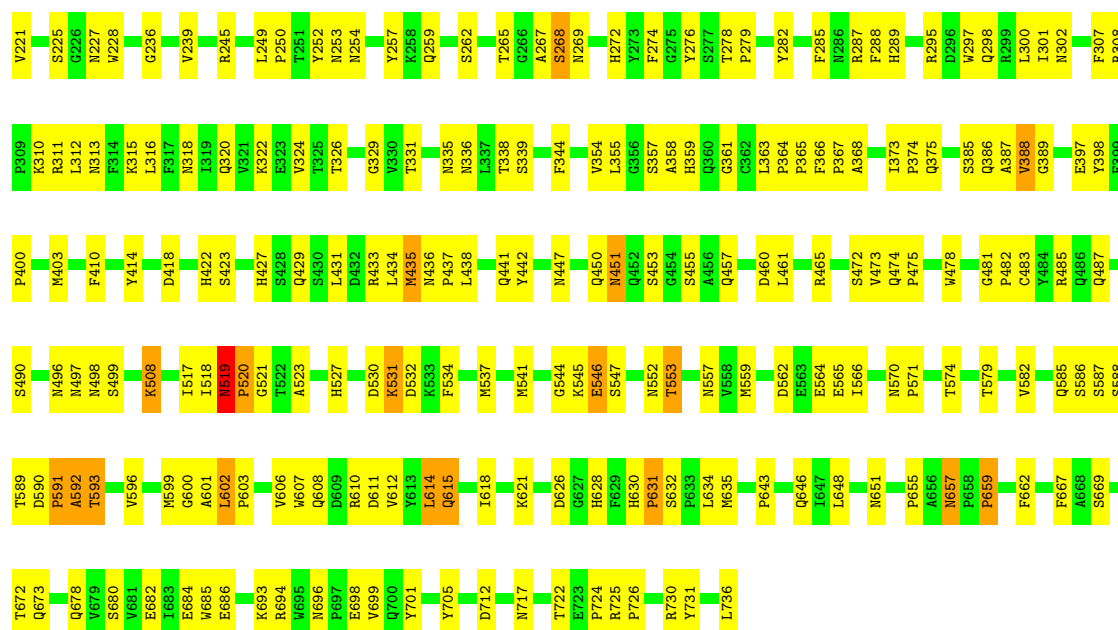
• Molecule 1: Capsid protein VP1

Chain Q:  59% 38%



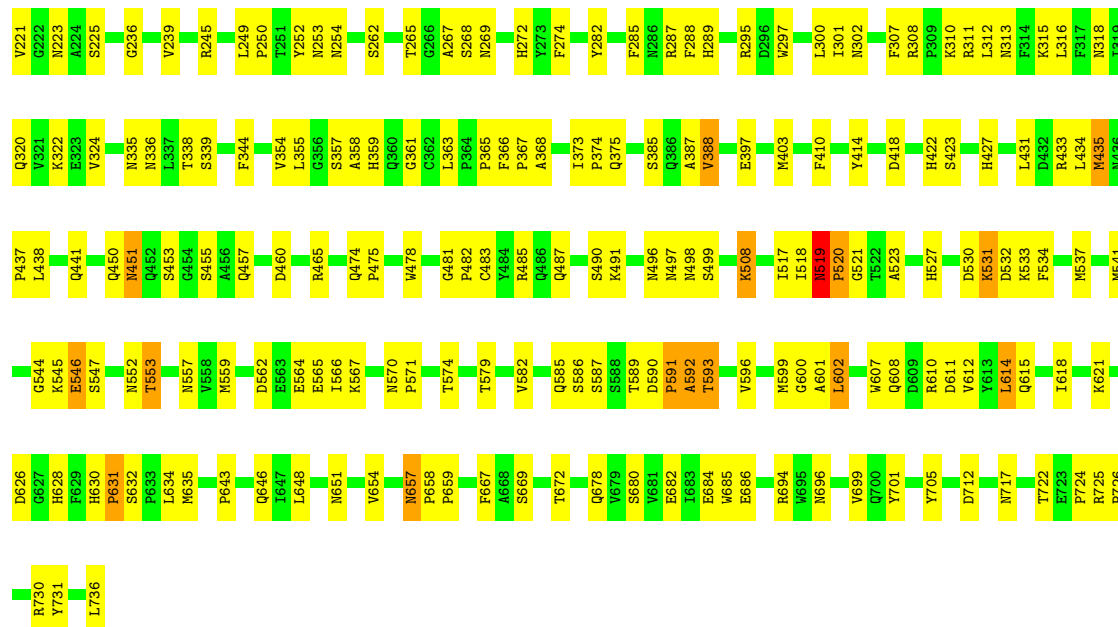
• Molecule 1: Capsid protein VP1

Chain R:  58% 38%



• Molecule 1: Capsid protein VP1

Chain S:  63% 34%



• Molecule 1: Capsid protein VP1

Chain T:  60% 36%



R694	W695	N696	V699	Q700	Y701	Y705	D712	N717	T722	E723	P724	R725	P726	R730	Y731	L736	L602	W607	Q608	D609	R610	D611	V612	Y613	L614	Q615	I618	K621	I622	P623	H624	T625	D626	G627	H628	F629	H630	P631	S632	P633	L634	M635	P643	Q646	I647	L648	N651	V654	N657	P658	P659	F667	A668	S669	T672	Q678	V679	S680	V681	E682	I683	E684	W685	E686																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	258.36Å 258.36Å 612.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 3.02 48.67 – 3.02	Depositor EDS
% Data completeness (in resolution range)	23.0 (48.67-3.02) 23.0 (48.67-3.02)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.273 , 0.286 0.271 , 0.287	Depositor DCC
R_{free} test set	980 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.078 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.060 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.048 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.049 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.059 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.057 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.136 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	82000	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.24	0/4226	0.68	0/5762
1	B	0.24	0/4226	0.68	0/5762
1	C	0.24	0/4226	0.68	0/5762
1	D	0.24	0/4226	0.68	0/5762
1	E	0.24	0/4226	0.68	0/5762
1	F	0.24	0/4226	0.68	0/5762
1	G	0.24	0/4226	0.68	0/5762
1	H	0.24	0/4226	0.67	0/5762
1	I	0.24	0/4226	0.68	0/5762
1	J	0.24	0/4226	0.68	0/5762
1	K	0.24	0/4226	0.68	0/5762
1	L	0.24	0/4226	0.68	0/5762
1	M	0.24	0/4226	0.68	0/5762
1	N	0.24	0/4226	0.68	0/5762
1	O	0.24	0/4226	0.68	0/5762
1	P	0.24	0/4226	0.68	0/5762
1	Q	0.24	0/4226	0.68	0/5762
1	R	0.24	0/4226	0.68	0/5762
1	S	0.24	0/4226	0.68	0/5762
1	T	0.24	0/4226	0.68	0/5762
All	All	0.24	0/84520	0.68	0/115240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4100	0	3881	149	1
1	B	4100	0	3881	179	2
1	C	4100	0	3881	145	2
1	D	4100	0	3881	185	1
1	E	4100	0	3881	187	1
1	F	4100	0	3881	225	0
1	G	4100	0	3881	187	1
1	H	4100	0	3881	218	0
1	I	4100	0	3881	217	1
1	J	4100	0	3881	205	2
1	K	4100	0	3881	179	1
1	L	4100	0	3881	180	2
1	M	4100	0	3881	150	5
1	N	4100	0	3881	217	0
1	O	4100	0	3881	183	2
1	P	4100	0	3881	214	0
1	Q	4100	0	3881	218	0
1	R	4100	0	3881	207	3
1	S	4100	0	3881	148	2
1	T	4100	0	3881	184	1
All	All	82000	0	77620	3202	15

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 20.

The worst 5 of 3202 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:J:658:PRO:HG2	1:L:250:PRO:HB3	1.19	1.14
1:J:705:TYR:O	1:R:388:VAL:HG12	1.59	1.03
1:J:397:GLU:HB2	1:L:367:PRO:HB2	1.45	0.98
1:D:359:HIS:HE1	1:E:436:ASN:H	1.03	0.96
1:B:359:HIS:HE1	1:G:436:ASN:H	1.01	0.95

The worst 5 of 15 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:I:454:GLY:O	1:O:668:ALA:O[3_545]	1.88	0.32
1:M:453:SER:OG	1:R:326:THR:OG1[4_455]	1.94	0.26
1:G:626:ASP:OD1	1:M:423:SER:OG[2_555]	2.07	0.13
1:B:423:SER:OG	1:M:626:ASP:OD1[2_555]	2.09	0.11
1:M:452:GLN:O	1:R:329:GLY:CA[4_455]	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	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	B	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	C	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	D	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	2	13
1	E	514/516 (100%)	438 (85%)	55 (11%)	21 (4%)	2	12
1	F	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	G	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	H	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	I	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	J	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	K	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	L	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	2	13
1	M	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	2	13
1	N	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	O	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	P	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	Q	514/516 (100%)	438 (85%)	55 (11%)	21 (4%)	2	12
1	R	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
1	T	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	2	13
All	All	10280/10320 (100%)	8756 (85%)	1122 (11%)	402 (4%)	2	13

5 of 402 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ALA
1	A	519	ASN
1	A	531	LYS
1	A	552	ASN
1	A	586	SER

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	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	B	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	C	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	D	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	E	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	F	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	G	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	H	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	I	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	J	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	K	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	L	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	M	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	N	451/451 (100%)	436 (97%)	15 (3%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	P	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	Q	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	R	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	S	451/451 (100%)	436 (97%)	15 (3%)	33	65
1	T	451/451 (100%)	436 (97%)	15 (3%)	33	65
All	All	9020/9020 (100%)	8720 (97%)	300 (3%)	33	65

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	519	ASN
1	T	295	ARG
1	P	657	ASN
1	R	508	LYS
1	G	593	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 514 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	223	ASN
1	S	452	GLN
1	R	704	ASN
1	H	487	GLN
1	H	350	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 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

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	516/516 (100%)	-1.88	0 100 100	72, 88, 112, 147	0
1	B	516/516 (100%)	-1.84	0 100 100	71, 87, 112, 144	0
1	C	516/516 (100%)	-1.84	0 100 100	70, 87, 110, 145	0
1	D	516/516 (100%)	-1.85	0 100 100	71, 88, 112, 144	0
1	E	516/516 (100%)	-1.84	0 100 100	71, 87, 111, 148	0
1	F	516/516 (100%)	-1.85	0 100 100	70, 87, 111, 147	0
1	G	516/516 (100%)	-1.85	0 100 100	73, 87, 112, 145	0
1	H	516/516 (100%)	-1.85	0 100 100	70, 86, 112, 145	0
1	I	516/516 (100%)	-1.84	0 100 100	71, 87, 112, 146	0
1	J	516/516 (100%)	-1.88	0 100 100	73, 89, 112, 147	0
1	K	516/516 (100%)	-1.85	0 100 100	70, 88, 113, 146	0
1	L	516/516 (100%)	-1.87	0 100 100	73, 88, 112, 146	0
1	M	516/516 (100%)	-1.86	0 100 100	70, 88, 112, 145	0
1	N	516/516 (100%)	-1.85	0 100 100	71, 87, 111, 146	0
1	O	516/516 (100%)	-1.85	0 100 100	70, 87, 111, 147	0
1	P	516/516 (100%)	-1.86	0 100 100	67, 86, 111, 146	0
1	Q	516/516 (100%)	-1.85	0 100 100	70, 87, 111, 146	0
1	R	516/516 (100%)	-1.88	0 100 100	72, 88, 112, 146	0
1	S	516/516 (100%)	-1.86	0 100 100	71, 87, 111, 145	0
1	T	516/516 (100%)	-1.85	0 100 100	72, 87, 111, 145	0
All	All	10320/10320 (100%)	-1.86	0 100 100	67, 87, 112, 148	0

There are no RSRZ outliers to report.

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.