



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:40 PM GMT

PDB ID : 3SHM
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 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>

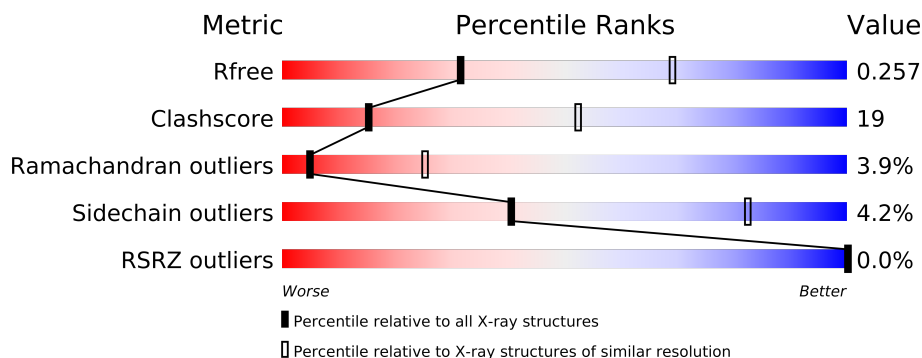
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.02 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}	66092	1332 (3.04-3.00)
Clashscore	79885	1732 (3.04-3.00)
Ramachandran outliers	78287	1669 (3.04-3.00)
Sidechain outliers	78261	1672 (3.04-3.00)
RSRZ outliers	66119	1333 (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 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	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	B	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	C	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	D	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	E	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	F	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	G	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	H	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	I	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	J	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	K	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	L	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	M	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	N	516	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
1	O	516	
1	P	516	
1	Q	516	
1	R	516	
1	S	516	
1	T	516	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 82000 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 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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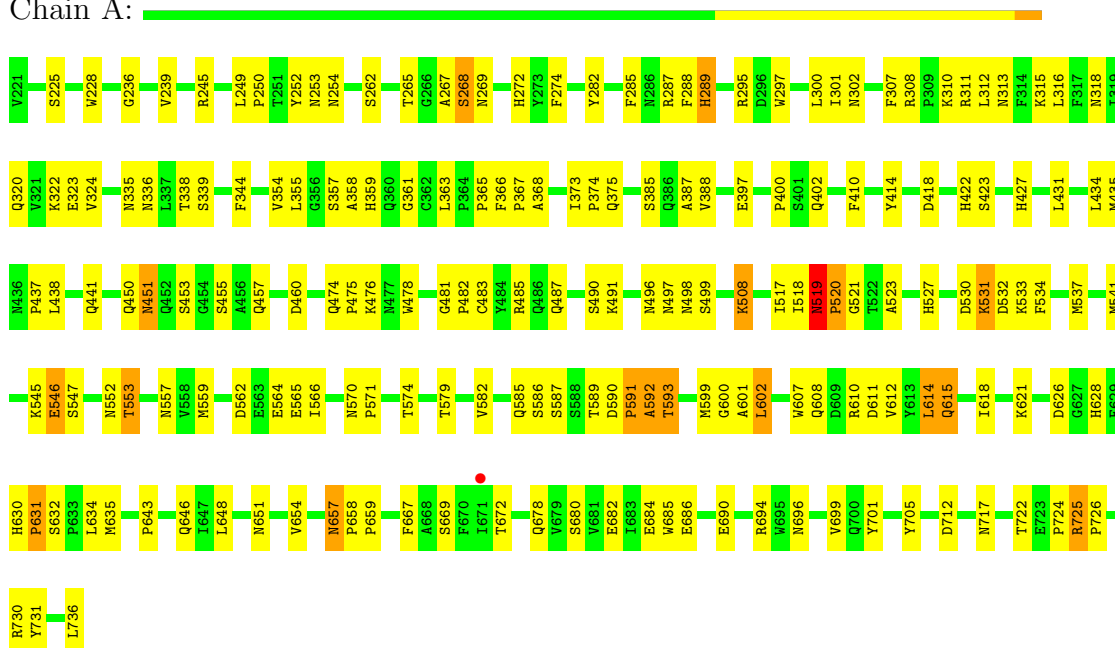
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0
1	R	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0
1	S	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0
1	T	516	Total 4100	C 2596	N 708	O 780	S 16	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA 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.

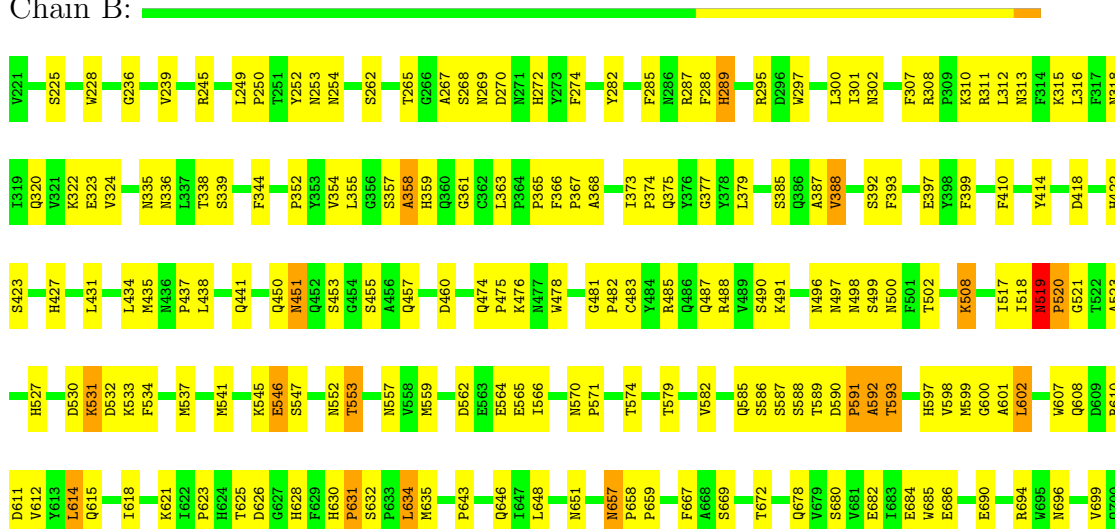
• Molecule 1: Capsid protein VP1

Chain A:



• Molecule 1: Capsid protein VP1

Chain B:



V699 Q700 Y701 Y705 D712 N717 T722 E723 P724 R725 P726 R730 Y731 L736

• Molecule 1: Capsid protein VP1

Chain H:

V221 S225 G236 V239 R245 L249 P250 T251 Y252 N253 N254 S262 T265 G266 A267 S268 N269 D270 N271 H272 Y273 F274 Y282 F285 N286 R287 F288 H289 R295 D296 W297 Q298 R299 L300 L301 N302 F307 R308 P309 K310 R311 L312 N313 F314 K315 L316 F317 N318 I319 Q320 V321 K322 E323 V324 N335 R336 L337 T338 S339 F344 V354 L355 G356 G357 A358 H359 Q360 G361 C362 L363 S364 P365 F366 P367 A368 I373 P374 Q375 Y376 G377 Y378 L379 S385 Q386 A387 V388 S392 F393 E397 Y398 F399 P400 F410 N496 N497 N498 N499 N500 F501 T502 S423 K508 I517 I518 H519 P520 G521 T522 A523 H527 D530 K531 D532 K533 F534 M537 H541 K545 E546 G547 S547 N552 T553 N557 P558 M559 D562 E563 E564 E565 I566 K567 N570 P571 T574 T579 V582 N583 L584 D585 S586 S587 S588 T589 D590 P591 A592 T593 H597 V598 M599 G600 A601 P603 V606 V607 Q608 D609 R610 D611 V612 V613 Q615 I618 K621 T625 D626 H628 F629 H630 Y731 L732 T733 L736 E684 M685 E686 E690 N691 S692 K693 R694 N695 P697 E698 V699 Q700 Y701 Y705 N717 T722 R725 P726 R730 Y731 L732 T733 L736

• Molecule 1: Capsid protein VP1

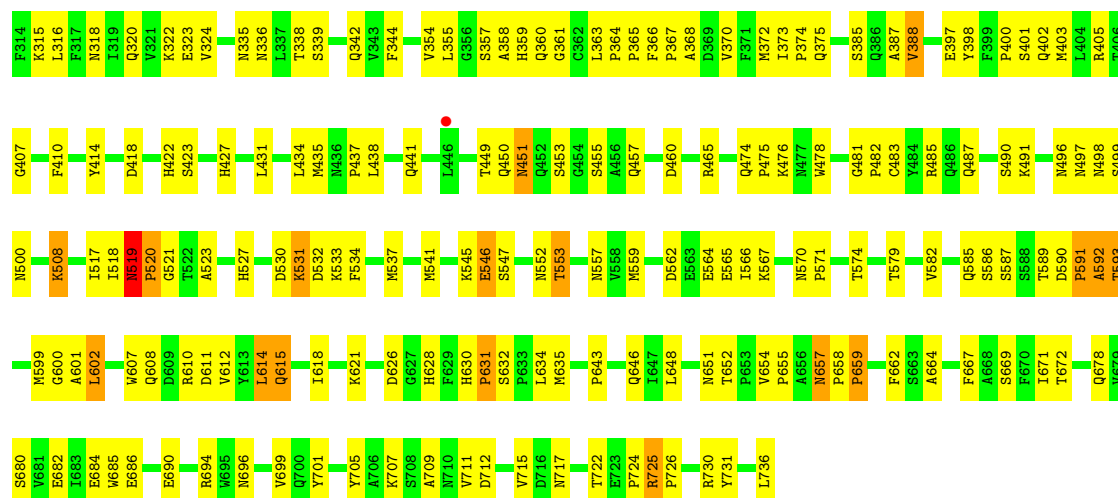
Chain I:

V221 S225 W228 G236 V239 R245 L249 P250 T251 Y252 N253 N254 S262 T265 G266 A267 S268 N269 D270 N271 H272 Y273 F274 Y282 F285 N286 R287 F288 H289 R295 D296 W297 Q298 R299 L300 L301 N302 F307 R308 P309 K310 R311 L312 N313 F314 K315 L316 F317 N318 I319 Q320 V321 K322 E323 V324 N335 R336 L337 T338 S339 F344 V354 L355 G356 G357 A358 H359 Q360 G361 C362 L363 S364 P365 F366 P367 A368 I373 P374 Q375 Y376 G377 Y378 L379 S385 Q386 A387 V388 S392 F393 E397 Y398 F399 P400 F410 N496 N497 N498 N499 N500 F501 T502 S423 K508 I517 I518 H519 P520 G521 T522 A523 H527 D530 K531 D532 K533 F534 M537 H541 K545 E546 G547 S547 N552 T553 N557 P558 M559 D562 E563 E564 E565 I566 K567 N570 P571 T574 T579 V582 N583 L584 D585 S586 S587 S588 T589 D590 P591 A592 T593 H597 V598 M599 G600 A601 P603 V606 V607 Q608 D609 R610 D611 V612 V613 Q615 I618 K621 T625 D626 H628 F629 H630 Y731 L732 T733 L736 E684 M685 E686 E690 N691 S692 K693 R694 N695 P697 E698 V699 Q700 Y701 Y705 N717 T722 R725 P726 R730 Y731 L732 T733 L736

• Molecule 1: Capsid protein VP1

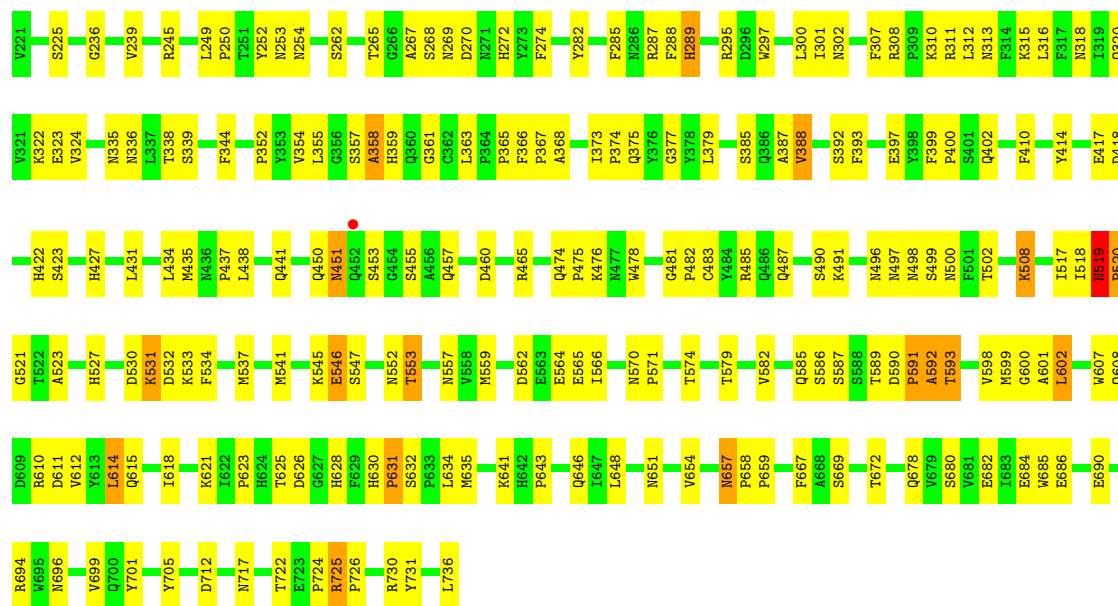
Chain J:

V221 S225 W228 D231 G236 V239 R245 L249 P250 T251 Y252 N253 N254 S262 T265 G266 A267 S268 N269 D270 N271 H272 Y273 F274 Y282 F285 N286 R287 F288 H289 R295 D296 W297 Q298 R299 L300 L301 N302 F307 R308 P309 K310 R311 L312 N313



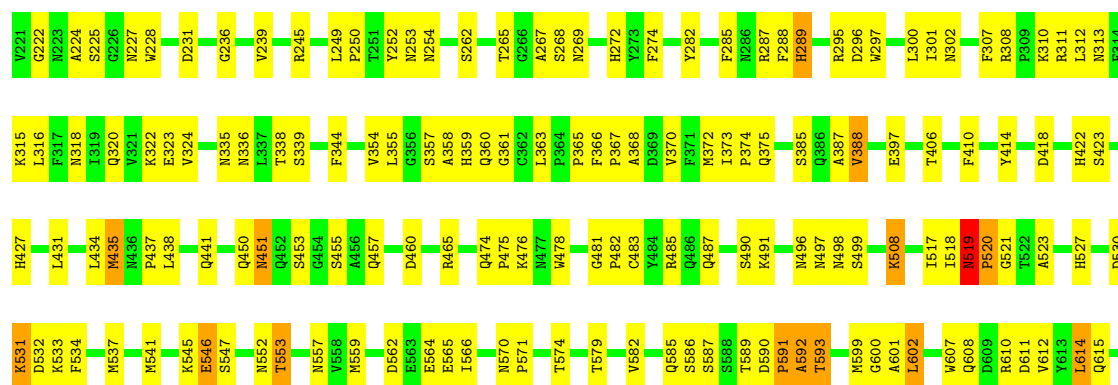
• Molecule 1: Capsid protein VP1

Chain K:



• Molecule 1: Capsid protein VP1

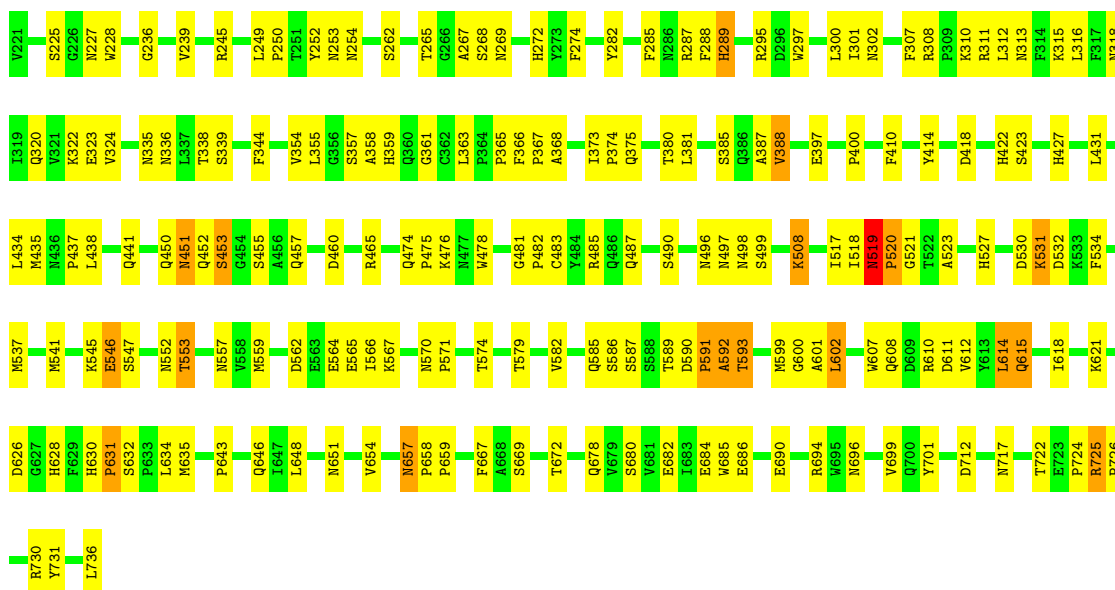
Chain L:





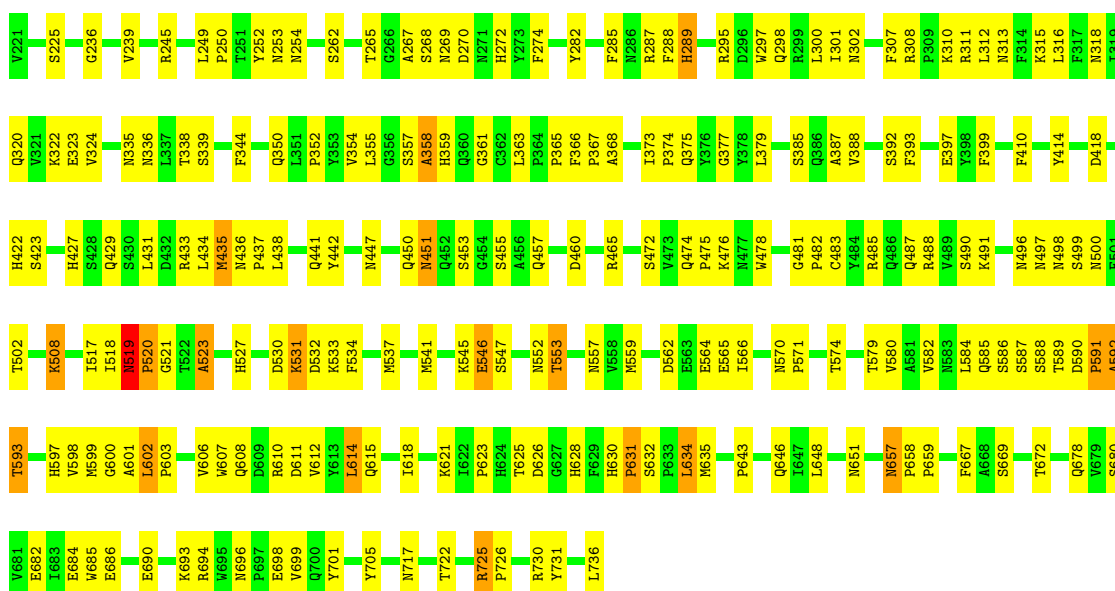
• Molecule 1: Capsid protein VP1

Chain M:



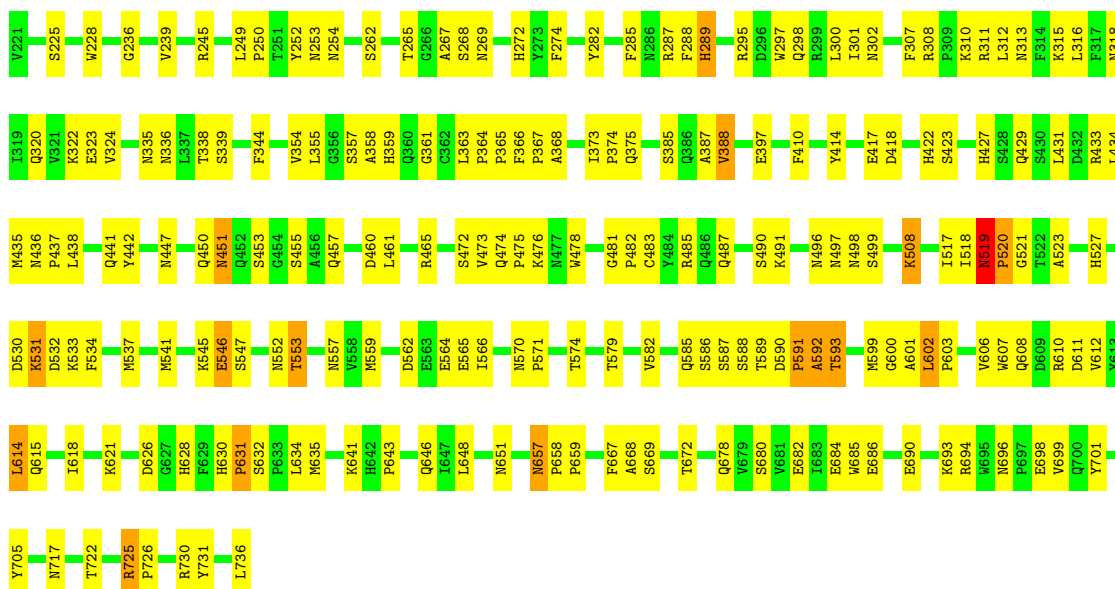
• Molecule 1: Capsid protein VP1

Chain N:



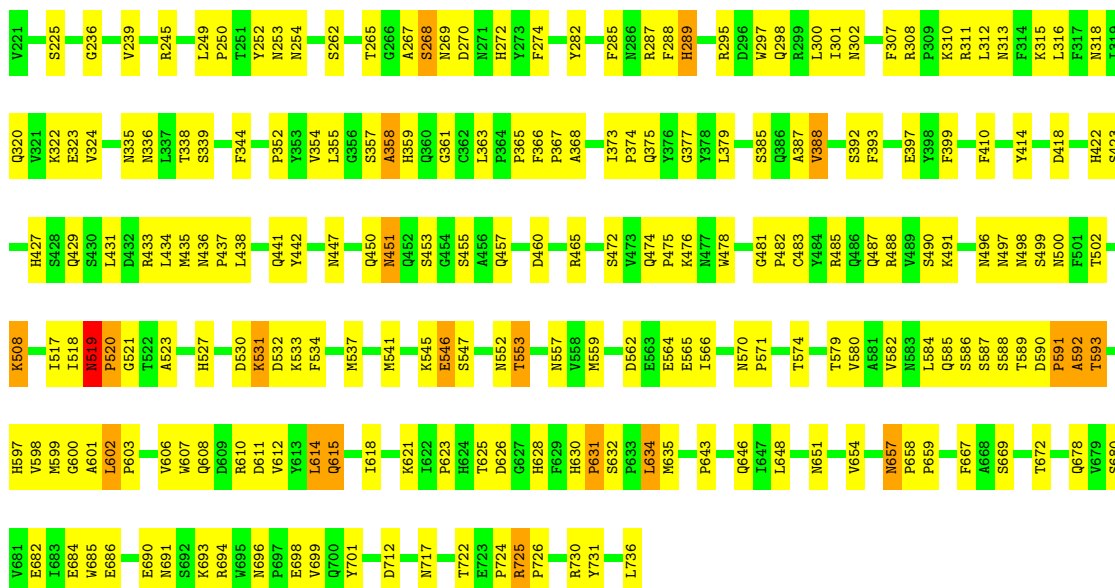
• Molecule 1: Capsid protein VP1

Chain O:



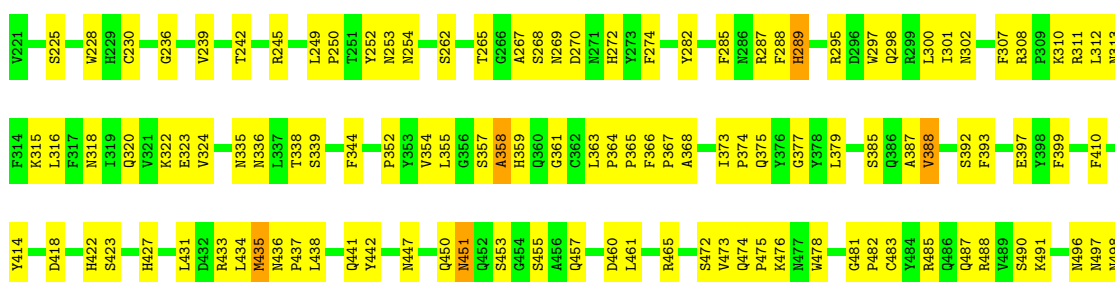
• Molecule 1: Capsid protein VP1

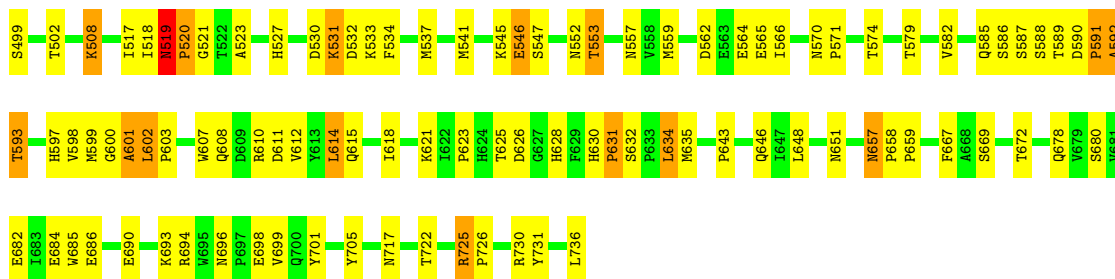
Chain P:



• Molecule 1: Capsid protein VP1

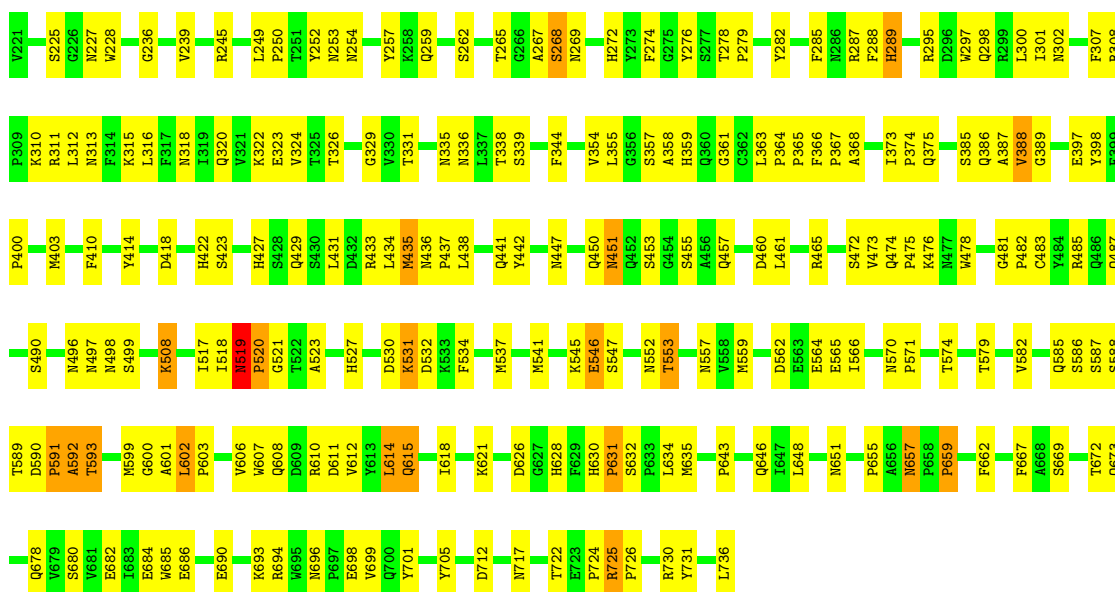
Chain Q:





• Molecule 1: Capsid protein VP1

Chain R:



N696	N610	T522	H422	I319	V221
V699	R610	A523	S423	Q320	S225
Q700	D611	H527	H427	V321	K322
Y701	V612	D530	L431	K324	E323
Y705	L613	K531	L434	N335	V228
D712	Q615	D532	M435	N336	Q236
N717	T618	F534	N436	L337	V239
T722	K621	M537	P437	T338	R245
E723	L622	M541	L438	S339	L249
P724	P623	K545	Q441	F344	P250
R725	T625	E546	Q450	P352	T251
P726	G627	S547	N451	Y353	Y252
R730	H628	S547	Q452	V354	N253
Y731	F629	N552	S453	L355	N254
L736	H630	T553	G454	G356	S262
	P631	N557	A456	S357	T265
	S632	V558	Q457	H359	A267
	L634	M559	D460	Q360	S268
	M635	D562	R465	G361	N269
	P643	E563	Q474	C362	D270
	Q646	E564	N477	L363	N271
	L648	I566	W478	P364	H272
	N651	N570	G481	P366	V273
	V654	P571	P482	P367	F274
	N657	T574	C483	A368	Y282
	P658	T579	Y484	I373	F285
	P659	V582	R485	Q375	N286
	F667	Q585	Q486	G376	R287
	A668	S586	Q487	G377	F288
	S669	S587	S490	L379	H289
	T672	S588	K491	S385	R295
	D678	T589	N496	Q386	D296
	V679	D590	N497	A387	W297
	S680	P591	N498	V388	L300
	V681	A592	S499	S392	I301
	E682	T593	N500	F393	N302
	T683	H597	F501	E397	F307
	E684	V598	T502	Y398	R308
	M685	M599	K508	F399	F309
	E686	G600	F517	P400	K310
	E690	A601	T518	F410	R311
	R694	L602	N519	Y414	L312
	W695	W607	P520	Y418	N313
		Q608	G521	D418	F314
					K315
					L316
					F317
					N318

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 (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.273 , 0.286 0.241 , 0.257	Depositor DCC
R_{free} test set	977 reflections (1.42%)	DCC
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.5	EDS
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
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 68828 reflections	Xtriage
F_o, F_c correlation	0.87	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/4226	0.37	0/5762
1	B	0.21	0/4226	0.37	0/5762
1	C	0.21	0/4226	0.37	0/5762
1	D	0.22	0/4226	0.37	0/5762
1	E	0.21	0/4226	0.37	0/5762
1	F	0.21	0/4226	0.37	0/5762
1	G	0.21	0/4226	0.37	0/5762
1	H	0.22	0/4226	0.37	0/5762
1	I	0.22	0/4226	0.37	0/5762
1	J	0.22	0/4226	0.37	0/5762
1	K	0.21	0/4226	0.37	0/5762
1	L	0.22	0/4226	0.37	0/5762
1	M	0.22	0/4226	0.37	0/5762
1	N	0.21	0/4226	0.37	0/5762
1	O	0.21	0/4226	0.37	0/5762
1	P	0.22	0/4226	0.37	0/5762
1	Q	0.21	0/4226	0.37	0/5762
1	R	0.22	0/4226	0.37	0/5762
1	S	0.21	0/4226	0.37	0/5762
1	T	0.21	0/4226	0.37	0/5762
All	All	0.21	0/84520	0.37	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 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	4100	0	3881	137	1
1	B	4100	0	3881	167	2
1	C	4100	0	3881	133	2
1	D	4100	0	3881	170	1
1	E	4100	0	3881	173	1
1	F	4100	0	3881	213	0
1	G	4100	0	3881	174	1
1	H	4100	0	3881	208	0
1	I	4100	0	3881	207	1
1	J	4100	0	3881	194	2
1	K	4100	0	3881	166	1
1	L	4100	0	3881	167	2
1	M	4100	0	3881	137	5
1	N	4100	0	3881	204	0
1	O	4100	0	3881	168	2
1	P	4100	0	3881	204	0
1	Q	4100	0	3881	203	0
1	R	4100	0	3881	197	3
1	S	4100	0	3881	134	2
1	T	4100	0	3881	170	1
All	All	82000	0	77620	2997	15

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 19.

The worst 5 of 2997 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	B	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	C	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	D	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	5	25
1	E	514/516 (100%)	438 (85%)	55 (11%)	21 (4%)	4	23
1	F	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	G	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	H	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	I	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	J	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	K	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	L	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	5	25
1	M	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	5	25
1	N	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	O	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	P	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	Q	514/516 (100%)	438 (85%)	55 (11%)	21 (4%)	4	23
1	R	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	5	25
1	S	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25
1	T	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	10280/10320 (100%)	8756 (85%)	1122 (11%)	402 (4%)	5	25

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%)	432 (96%)	19 (4%)	40	82
1	B	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	C	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	D	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	E	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	F	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	G	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	H	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	I	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	J	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	K	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	L	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	M	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	N	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	O	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	P	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	Q	451/451 (100%)	432 (96%)	19 (4%)	40	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	S	451/451 (100%)	432 (96%)	19 (4%)	40	82
1	T	451/451 (100%)	432 (96%)	19 (4%)	40	82
All	All	9020/9020 (100%)	8640 (96%)	380 (4%)	40	82

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	289	HIS
1	L	388	VAL
1	S	593	THR
1	J	435	MET
1	K	323	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 464 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	651	ASN
1	L	302	ASN
1	S	342	GLN
1	J	302	ASN
1	K	313	ASN

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	516/516 (100%)	-0.05	1 (0%) 93 53	72, 88, 112, 147	0
1	B	516/516 (100%)	-0.02	0 100 100	71, 87, 112, 144	0
1	C	516/516 (100%)	0.00	0 100 100	70, 87, 110, 145	0
1	D	516/516 (100%)	-0.05	0 100 100	71, 88, 112, 144	0
1	E	516/516 (100%)	-0.05	0 100 100	71, 87, 111, 148	0
1	F	516/516 (100%)	-0.01	0 100 100	70, 87, 111, 147	0
1	G	516/516 (100%)	-0.06	0 100 100	73, 87, 112, 145	0
1	H	516/516 (100%)	0.00	0 100 100	70, 86, 112, 145	0
1	I	516/516 (100%)	-0.04	0 100 100	71, 87, 112, 146	0
1	J	516/516 (100%)	-0.09	1 (0%) 93 53	73, 89, 112, 147	0
1	K	516/516 (100%)	-0.05	1 (0%) 93 53	70, 88, 113, 146	0
1	L	516/516 (100%)	-0.08	0 100 100	73, 88, 112, 146	0
1	M	516/516 (100%)	-0.06	0 100 100	70, 88, 112, 145	0
1	N	516/516 (100%)	-0.02	0 100 100	71, 87, 111, 147	0
1	O	516/516 (100%)	-0.02	0 100 100	70, 87, 111, 147	0
1	P	516/516 (100%)	-0.01	0 100 100	67, 86, 111, 146	0
1	Q	516/516 (100%)	-0.01	0 100 100	70, 87, 111, 146	0
1	R	516/516 (100%)	-0.07	0 100 100	72, 88, 112, 146	0
1	S	516/516 (100%)	-0.05	0 100 100	71, 87, 111, 145	0
1	T	516/516 (100%)	-0.01	0 100 100	72, 87, 111, 145	0
All	All	10320/10320 (100%)	-0.04	3 (0%) 100 100	67, 87, 112, 148	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	ILE	2.5
1	K	452	GLN	2.2
1	J	446	LEU	2.0

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.