



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 06:00 PM BST

PDB ID : 3TSX
Title : Structure-function Analysis of Receptor-binding in Adeno-Associated Virus Serotype 6 (AAV-6)
Authors : Xie, Q.
Deposited on : 2011-09-13
Resolution : 3.00 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>

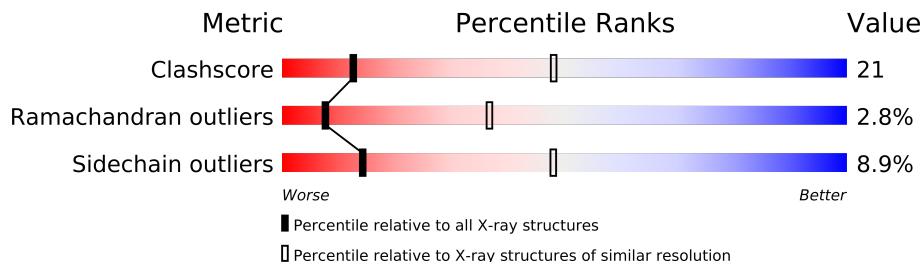
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)




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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	520	
1	B	520	
1	C	520	
1	D	520	
1	E	520	
1	F	520	
1	G	520	
1	H	520	
1	I	520	
1	J	520	
1	K	520	
1	L	520	
1	M	520	
1	N	520	
1	O	520	
1	P	520	
1	Q	520	

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Mol	Chain	Length	Quality of chain
1	R	520	
1	S	520	
1	T	520	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 82420 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	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	B	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	C	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	D	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	E	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	F	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	G	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	H	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	I	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	J	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	K	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	L	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	M	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	N	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	O	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	P	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	R	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	S	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	T	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0

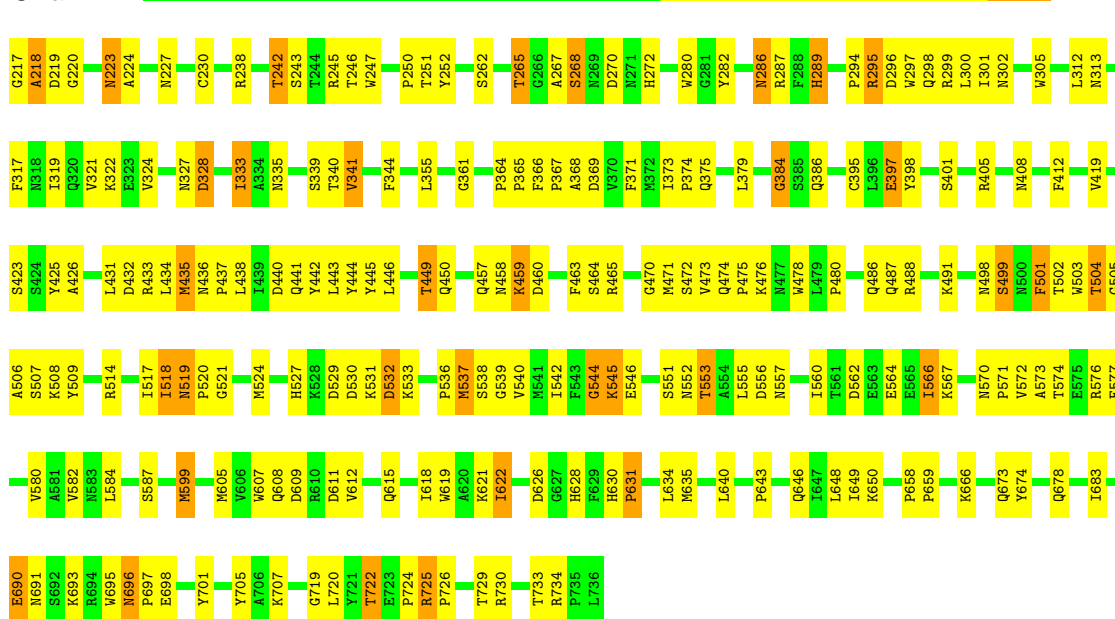
3 Residue-property plots

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.

Note EDS was not executed.

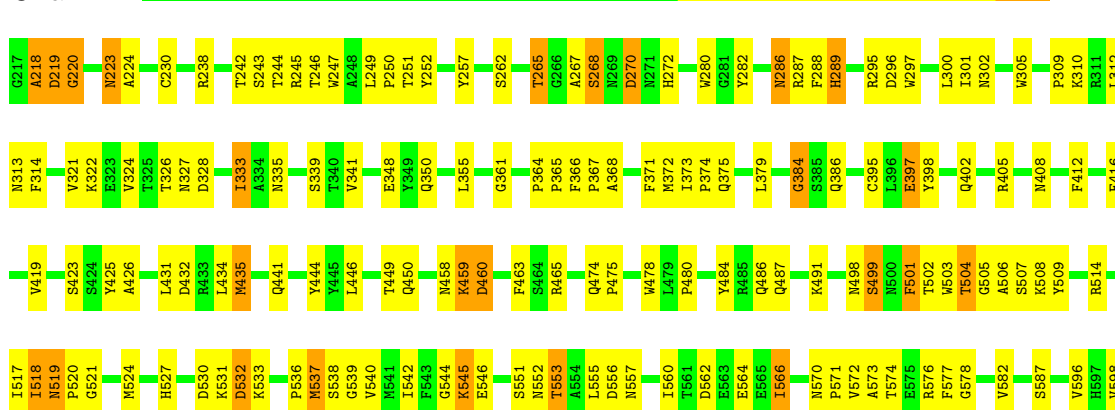
• Molecule 1: Capsid protein VP1

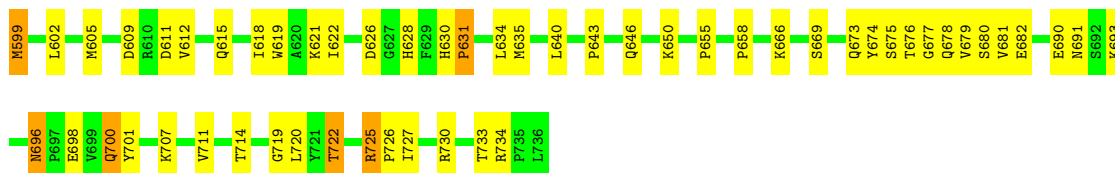
Chain A:



• Molecule 1: Capsid protein VP1

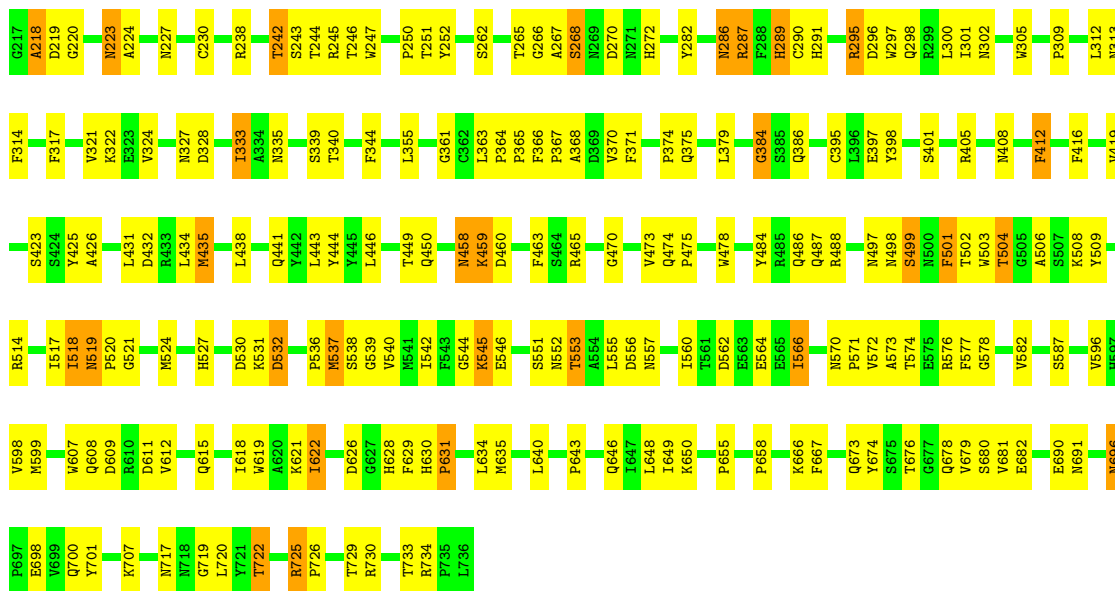
Chain B:





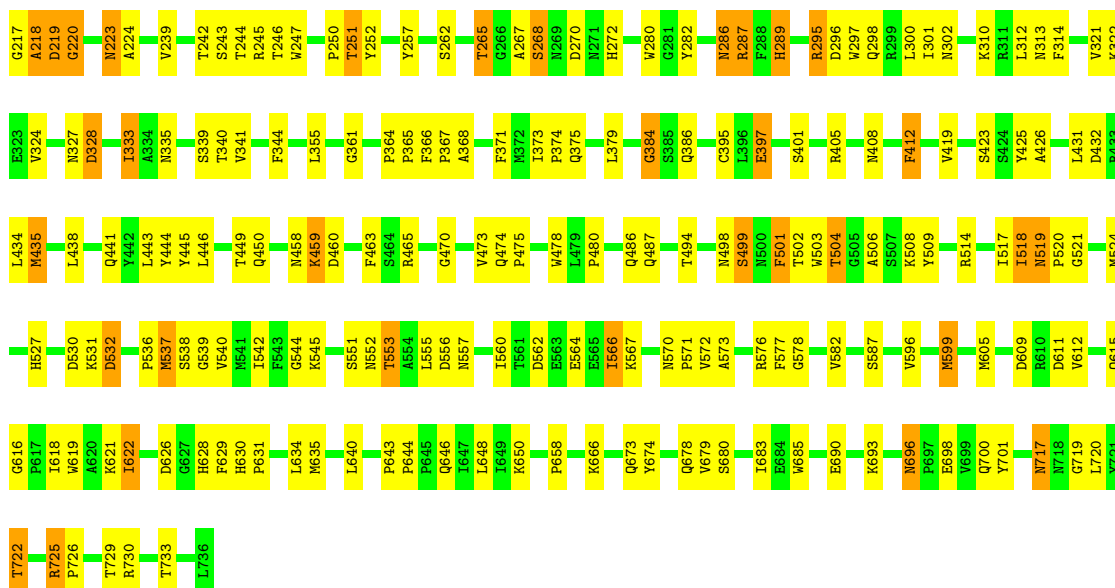
• Molecule 1: Capsid protein VP1

Chain C:



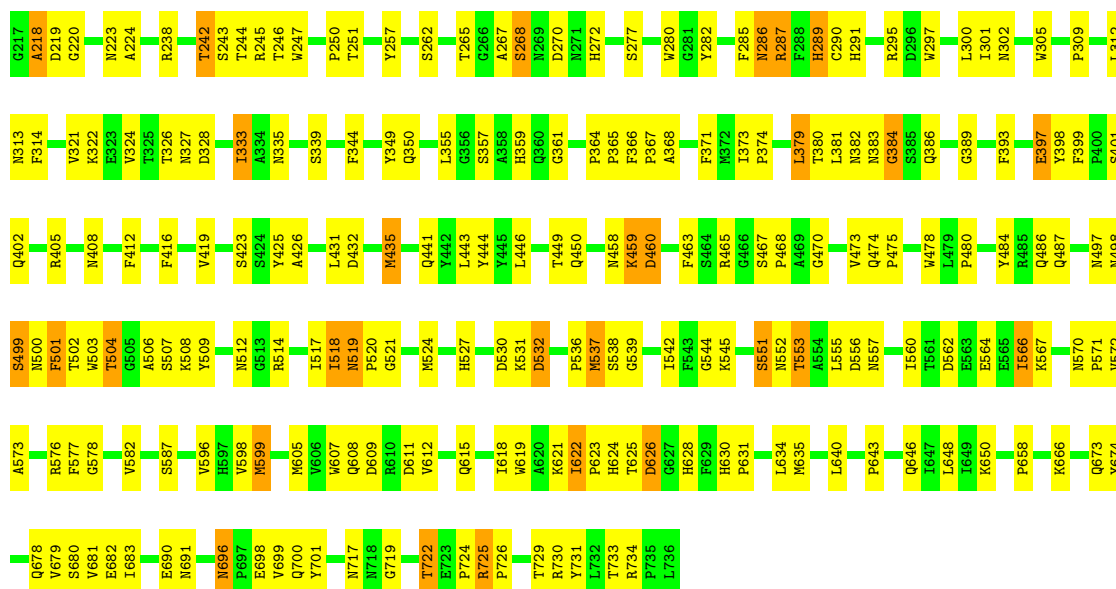
• Molecule 1: Capsid protein VP1

Chain D:



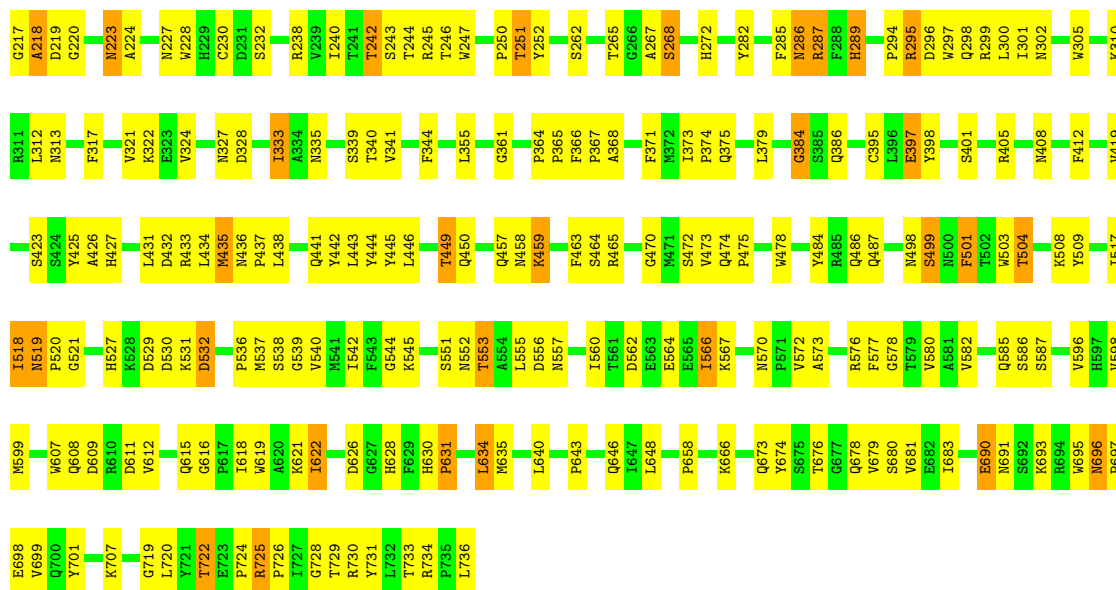
• Molecule 1: Capsid protein VP1

Chain E:



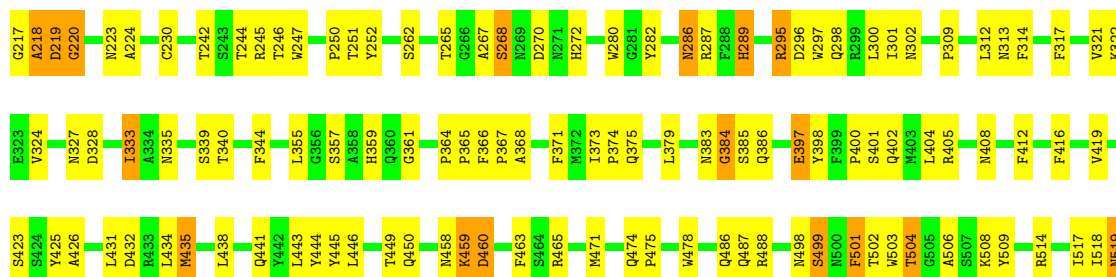
• Molecule 1: Capsid protein VP1

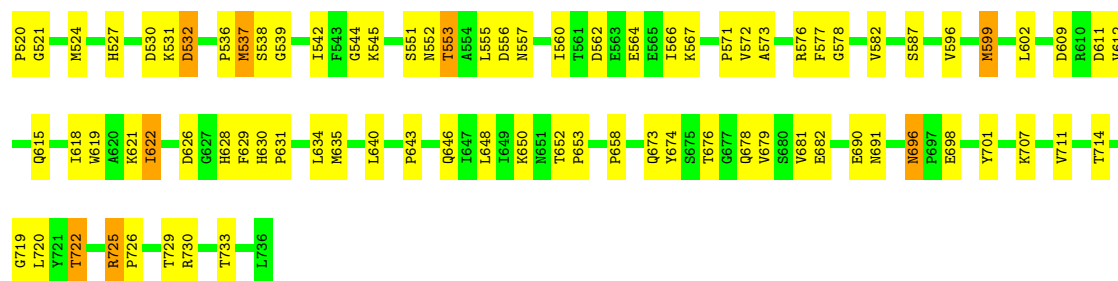
Chain F:



• Molecule 1: Capsid protein VP1

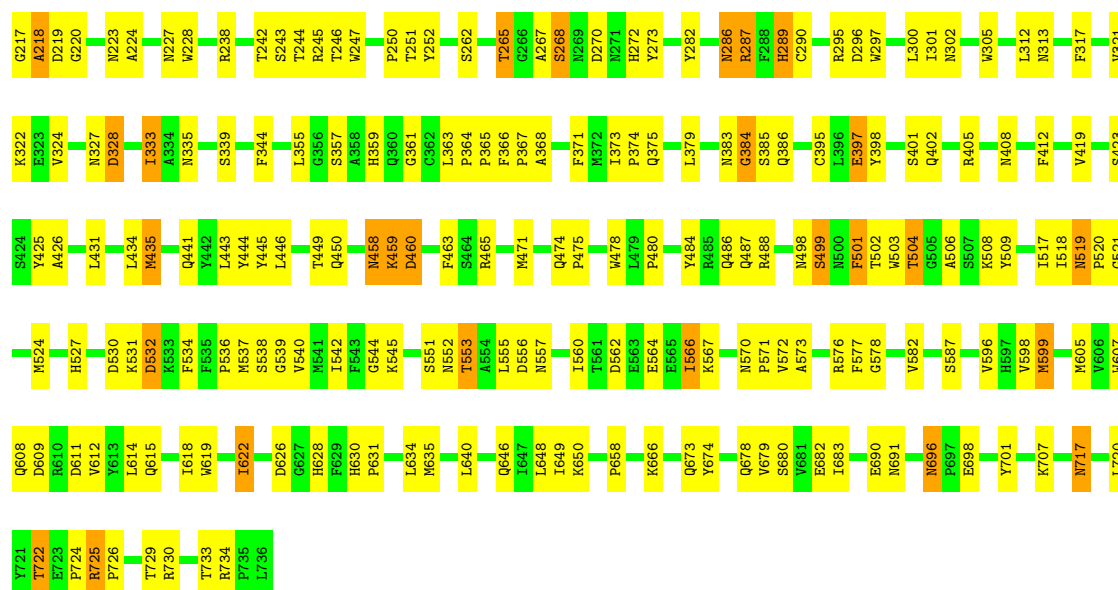
Chain G:





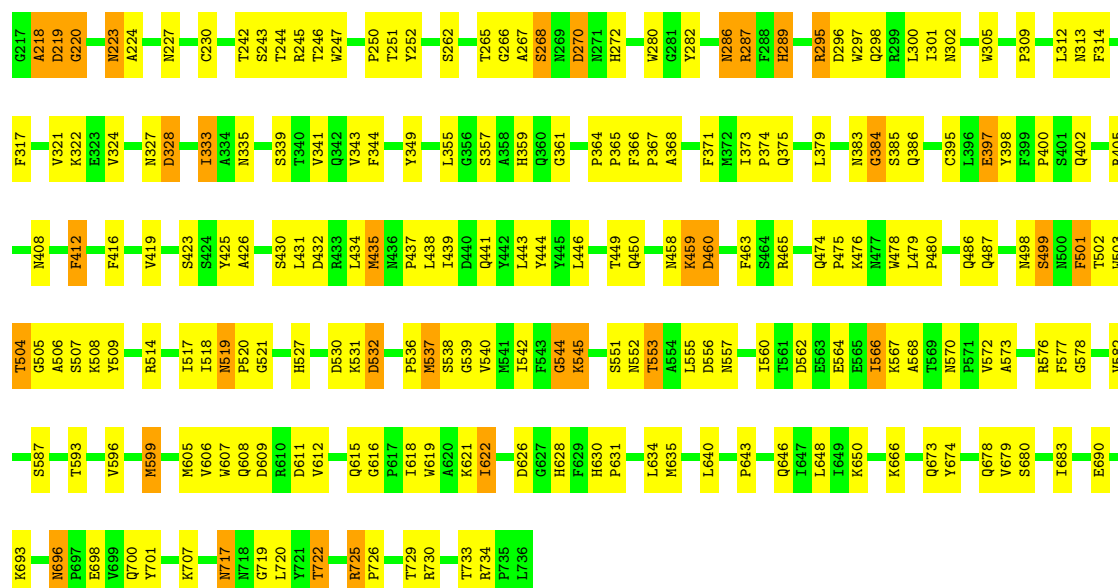
• Molecule 1: Capsid protein VP1

Chain H:

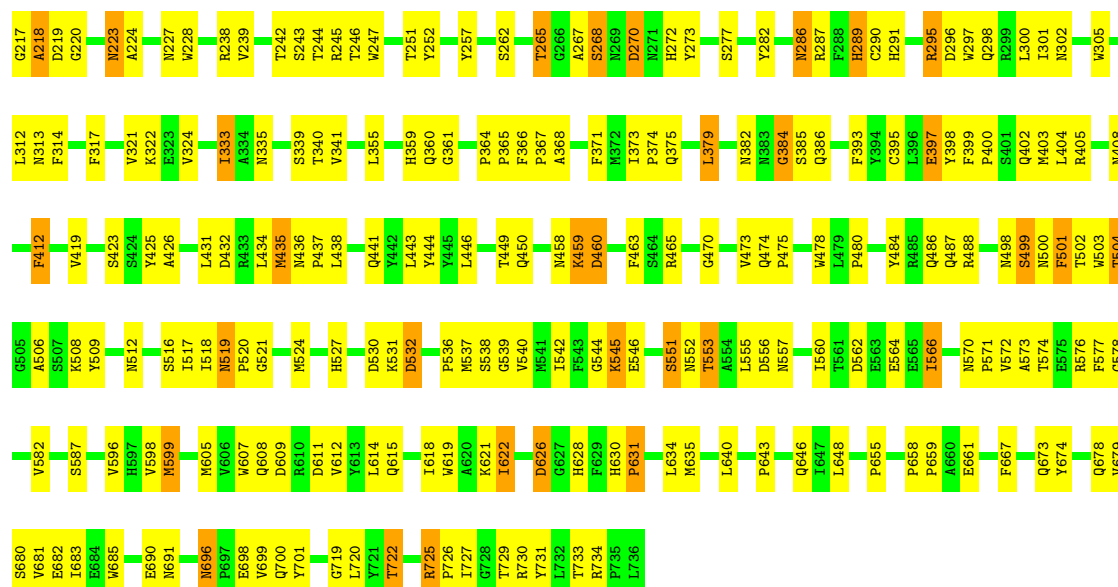


• Molecule 1: Capsid protein VP1

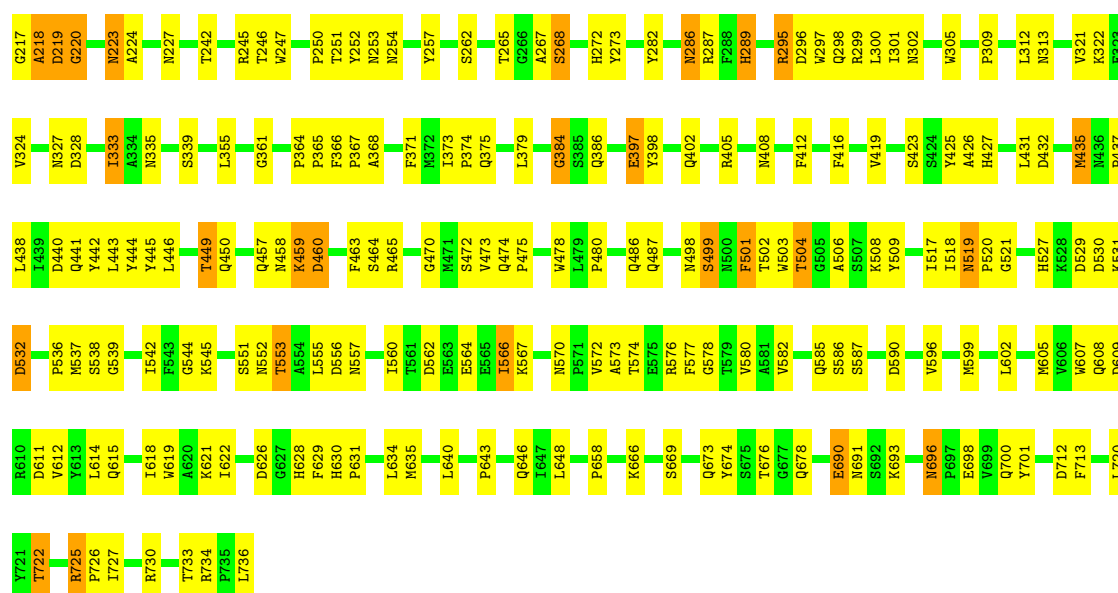
Chain I:



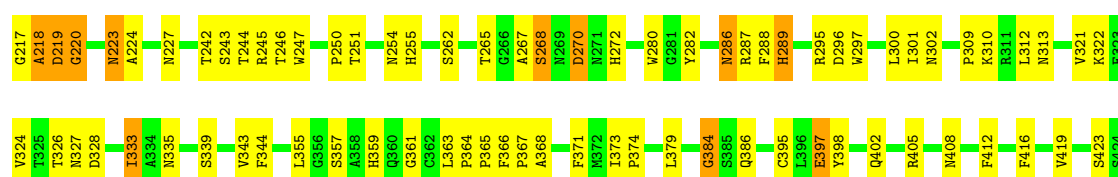
- Molecule 1: Capsid protein VP1

Chain J: 

- Molecule 1: Capsid protein VP1

Chain K: 

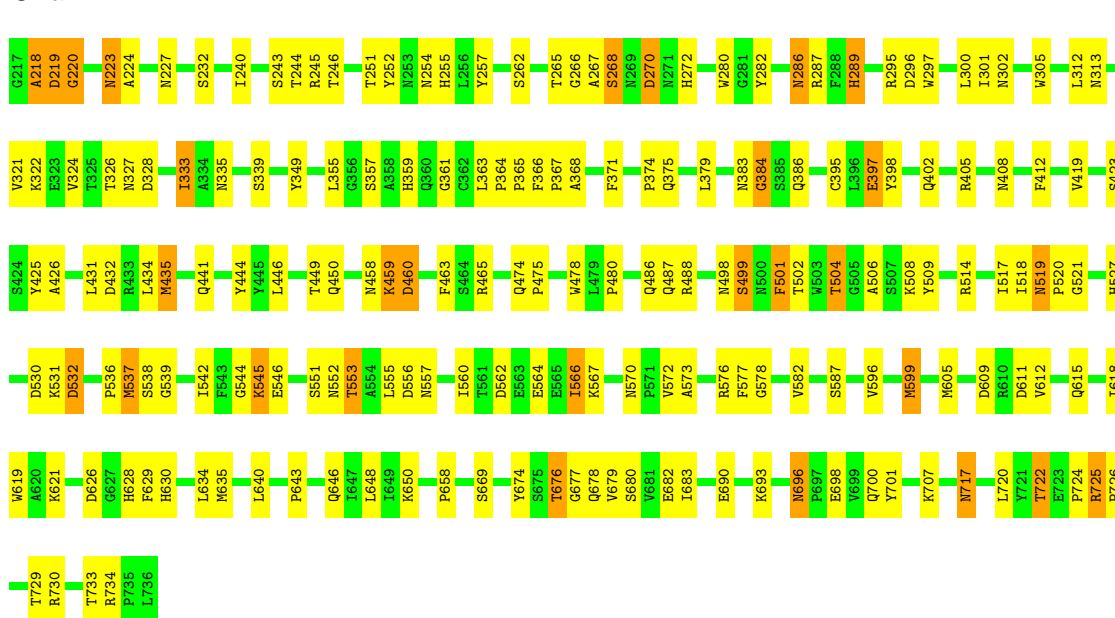
- Molecule 1: Capsid protein VP1

Chain L: 



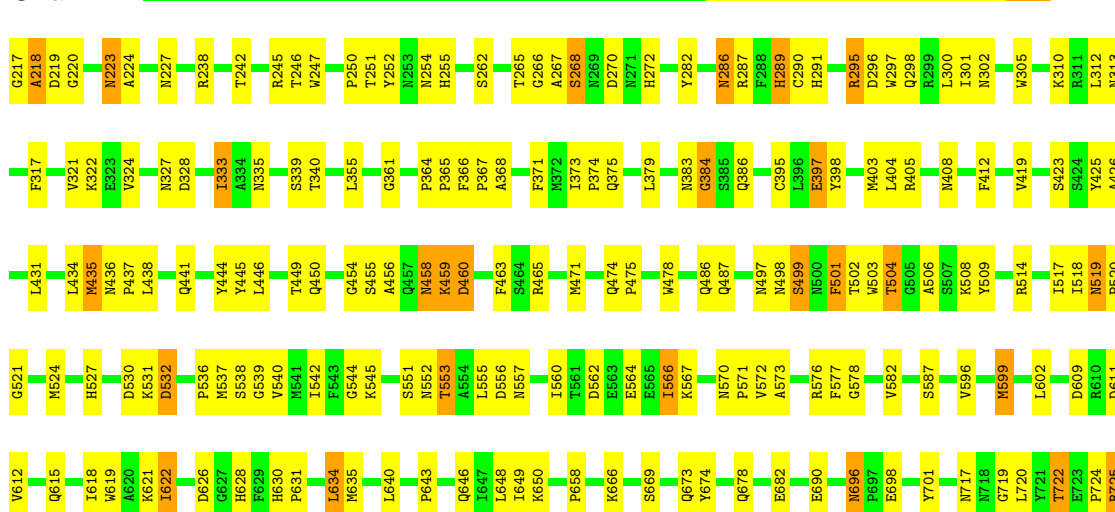
• Molecule 1: Capsid protein VP1

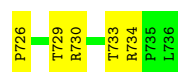
Chain M:



• Molecule 1: Capsid protein VP1

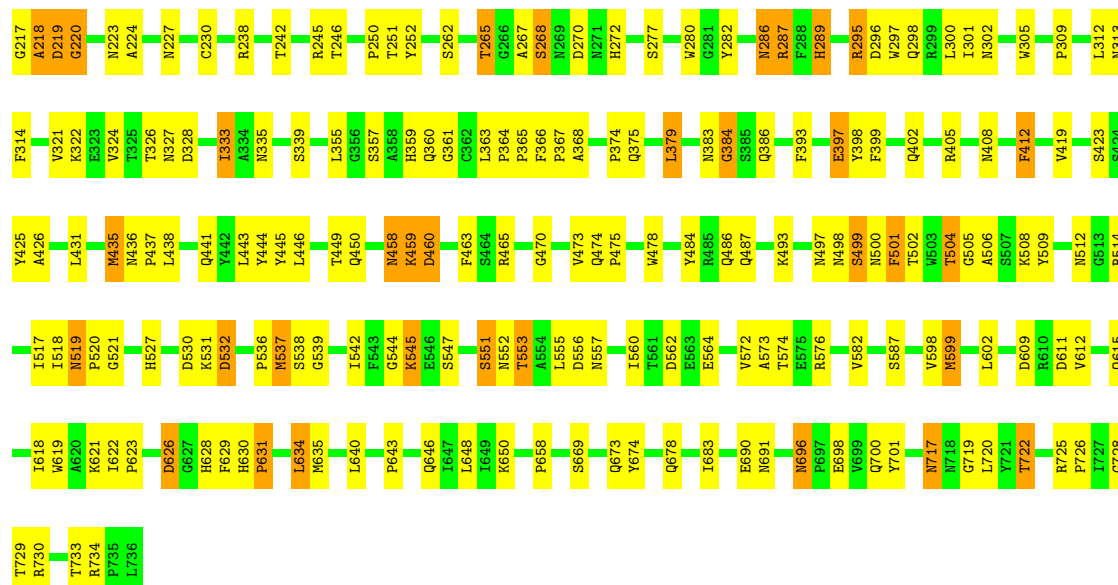
Chain N:





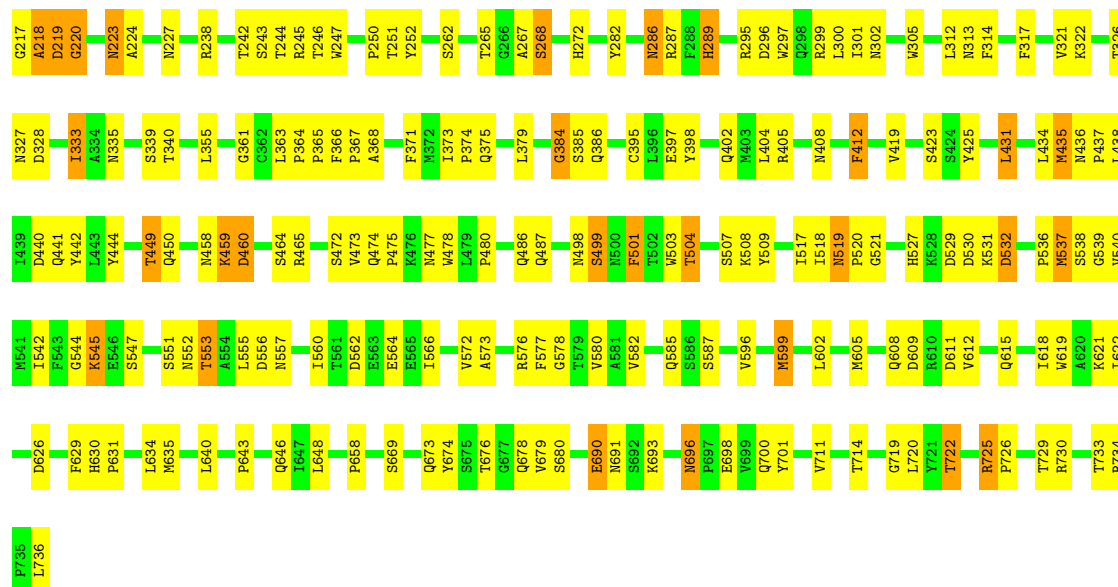
• Molecule 1: Capsid protein VP1

Chain O:



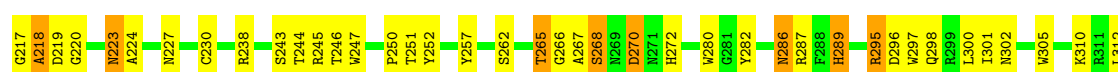
• Molecule 1: Capsid protein VP1

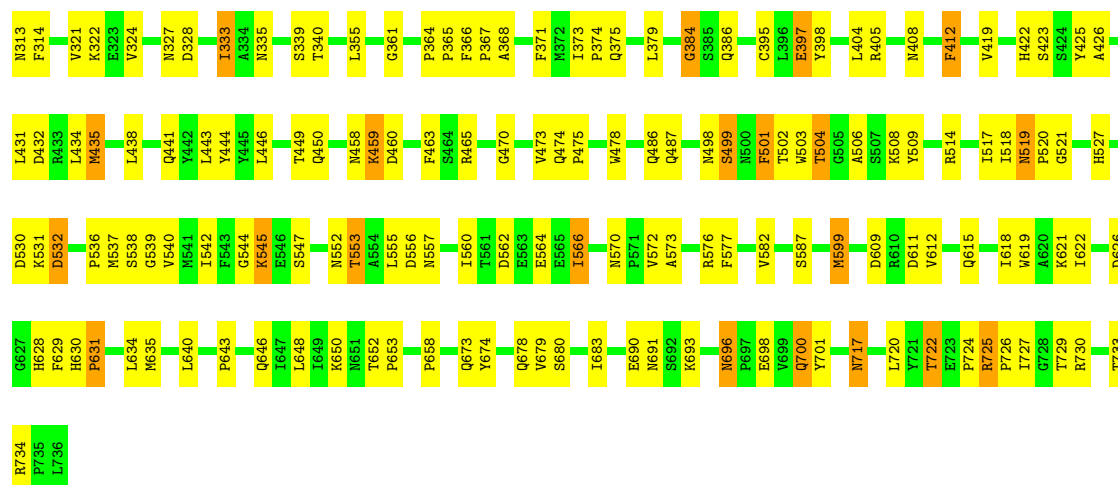
Chain P:



• Molecule 1: Capsid protein VP1

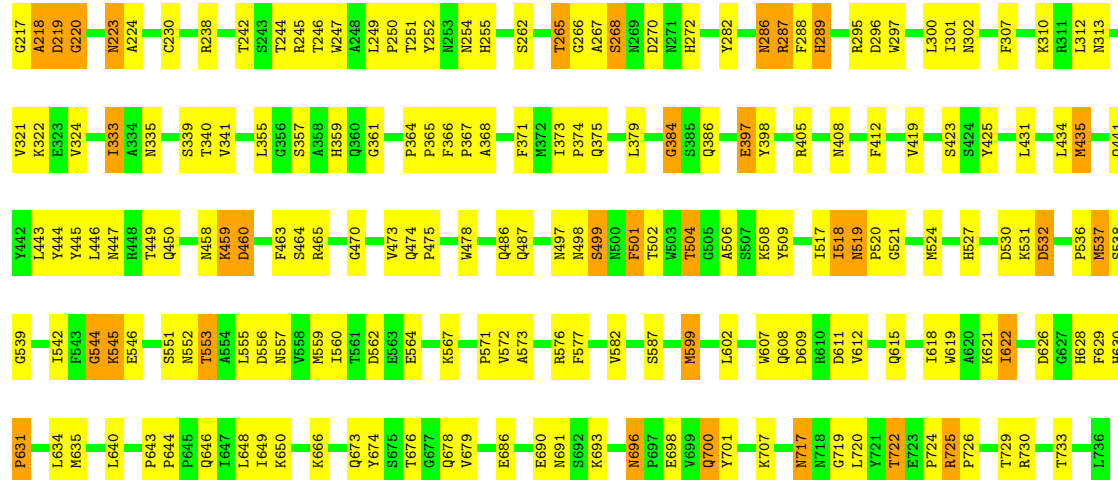
Chain Q:





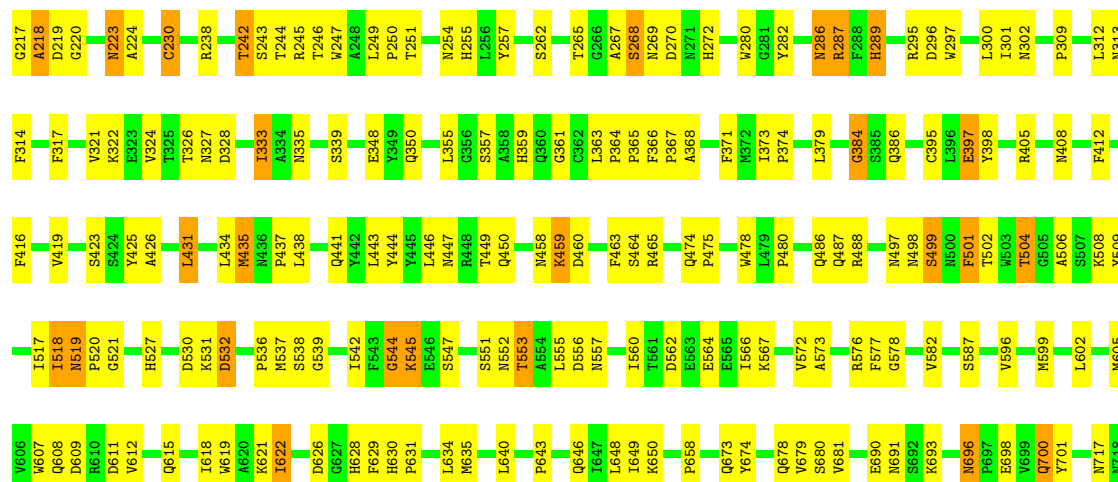
• Molecule 1: Capsid protein VP1

Chain R:



• Molecule 1: Capsid protein VP1

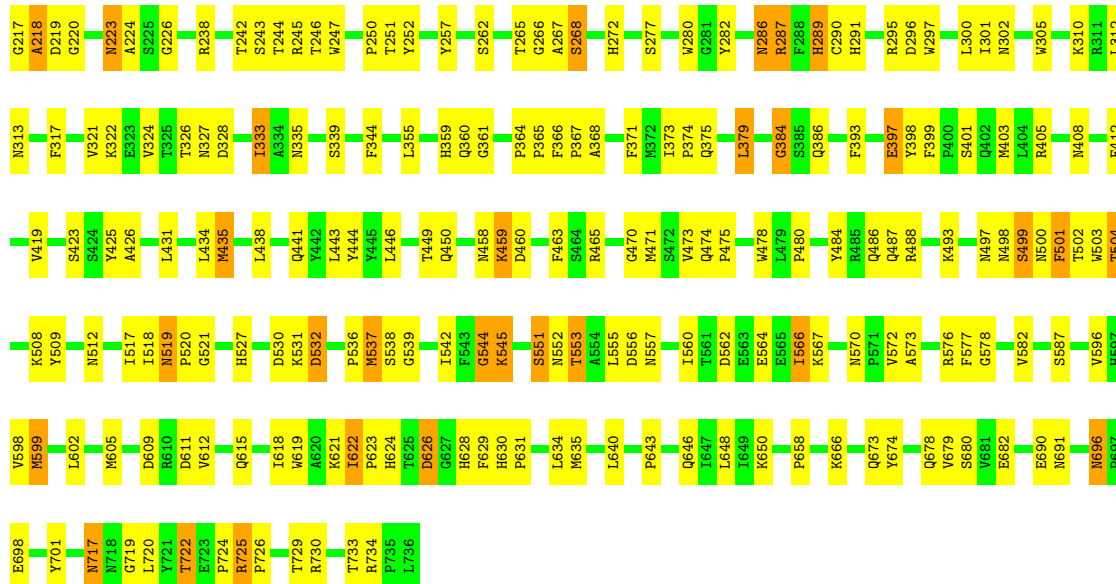
Chain S:





• Molecule 1: Capsid protein VP1

Chain T:



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	354.79Å 363.90Å 371.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.00	Depositor
% Data completeness (in resolution range)	35.1 (49.21-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.251 , 0.286	Depositor
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.389	Xtriage
Estimated twinning fraction	0.019 for -h,l,k 0.009 for -l,-k,-h 0.023 for k,h,-l 0.008 for k,l,h 0.008 for l,h,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 332221 reflections (0.000%)	Xtriage
Total number of atoms	82420	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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	0.68	0/4247	0.65	0/5790
1	B	0.66	0/4247	0.63	0/5790
1	C	0.58	0/4247	0.62	0/5790
1	D	0.60	2/4247 (0.0%)	0.63	2/5790 (0.0%)
1	E	0.65	0/4247	0.64	0/5790
1	F	0.62	0/4247	0.64	0/5790
1	G	0.58	0/4247	0.60	0/5790
1	H	0.56	0/4247	0.61	0/5790
1	I	0.65	0/4247	0.64	0/5790
1	J	0.70	0/4247	0.65	0/5790
1	K	0.58	0/4247	0.61	0/5790
1	L	0.55	0/4247	0.60	0/5790
1	M	0.55	0/4247	0.59	0/5790
1	N	0.57	0/4247	0.60	0/5790
1	O	0.56	1/4247 (0.0%)	0.60	0/5790
1	P	0.57	0/4247	0.62	0/5790
1	Q	0.56	0/4247	0.62	0/5790
1	R	0.56	0/4247	0.61	0/5790
1	S	0.63	1/4247 (0.0%)	0.62	0/5790
1	T	0.61	0/4247	0.61	0/5790
All	All	0.60	4/84940 (0.0%)	0.62	2/115800 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	230	CYS	CB-SG	-6.04	1.72	1.82
1	D	494	THR	CB-CG2	5.50	1.70	1.52
1	O	230	CYS	CB-SG	-5.44	1.73	1.81
1	D	494	THR	CA-CB	-5.10	1.40	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	494	THR	CA-CB-CG2	-5.89	104.15	112.40
1	D	494	THR	CB-CA-C	-5.82	95.88	111.60

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	4121	0	3896	241	0
1	B	4121	0	3896	185	0
1	C	4121	0	3896	175	0
1	D	4121	0	3896	165	0
1	E	4121	0	3896	228	0
1	F	4121	0	3896	238	0
1	G	4121	0	3896	166	0
1	H	4121	0	3896	180	0
1	I	4121	0	3896	181	0
1	J	4121	0	3896	231	0
1	K	4121	0	3896	201	4
1	L	4121	0	3896	169	0
1	M	4121	0	3896	158	0
1	N	4121	0	3896	163	5
1	O	4121	0	3896	188	0
1	P	4121	0	3896	197	0
1	Q	4121	0	3896	170	0
1	R	4121	0	3896	159	0
1	S	4121	0	3896	164	0
1	T	4121	0	3896	204	1
All	All	82420	0	77920	3371	5

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 21.

The worst 5 of 3371 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:464:SER:HB3	1:T:551:SER:HA	1.40	1.03
1:O:551:SER:HA	1:P:464:SER:HB3	1.41	1.03
1:T:562:ASP:OD1	1:T:564:GLU:OE2	1.82	0.97
1:A:696:ASN:HD21	1:J:393:PHE:H	1.08	0.96
1:S:408:ASN:HD21	1:T:224:ALA:H	1.13	0.95

All (5) 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:K:590:ASP:OD1	1:N:455:SER:N[4_556]	1.38	0.82
1:N:454:GLY:O	1:T:497:ASN:OD1[4_456]	1.71	0.49
1:K:590:ASP:OD2	1:N:455:SER:CB[4_556]	1.84	0.36
1:K:590:ASP:OD1	1:N:454:GLY:C[4_556]	2.07	0.13
1:K:590:ASP:OD1	1:N:455:SER:CA[4_556]	2.17	0.03

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	518/520 (100%)	460 (89%)	43 (8%)	15 (3%)	7	35
1	B	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	7	35
1	C	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	7	34
1	D	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	8	38
1	E	518/520 (100%)	463 (89%)	41 (8%)	14 (3%)	8	38
1	F	518/520 (100%)	462 (89%)	42 (8%)	14 (3%)	8	38
1	G	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	8	38
1	H	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	7	35
1	I	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	7	35
1	J	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	7	35
1	K	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	9	40
1	L	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	9	40
1	N	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	8	38
1	O	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	8	38
1	P	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	8	38
1	Q	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	8	38
1	R	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	7	34
1	S	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	9	40
1	T	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	9	40
All	All	10360/10400 (100%)	9297 (90%)	777 (8%)	286 (3%)	8	37

5 of 286 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	LYS
1	A	519	ASN
1	A	531	LYS
1	A	545	LYS
1	B	459	LYS

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	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	B	452/452 (100%)	409 (90%)	43 (10%)	12	44
1	C	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	D	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	E	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	F	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	G	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	H	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	I	452/452 (100%)	410 (91%)	42 (9%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	K	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	L	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	M	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	N	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	O	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	P	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	Q	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	R	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	S	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	T	452/452 (100%)	412 (91%)	40 (9%)	14	48
All	All	9040/9040 (100%)	8233 (91%)	807 (9%)	14	48

5 of 807 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	717	ASN
1	L	286	ASN
1	S	458	ASN
1	J	287	ARG
1	K	219	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 500 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	382	ASN
1	L	320	GLN
1	S	486	GLN
1	J	487	GLN
1	K	350	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.