



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:48 PM UTC

PDB ID : 2VF1 / pdb_00002vf1
Title : X-ray crystallographic structure of the picobirnavirus capsid
Authors : Duquerroy, S.; Da Costa, B.; Vigouroux, A.; Lepault, J.; Navaza, J.; Delmas, B.; Rey, F.A.
Deposited on : 2007-10-29
Resolution : 3.40 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

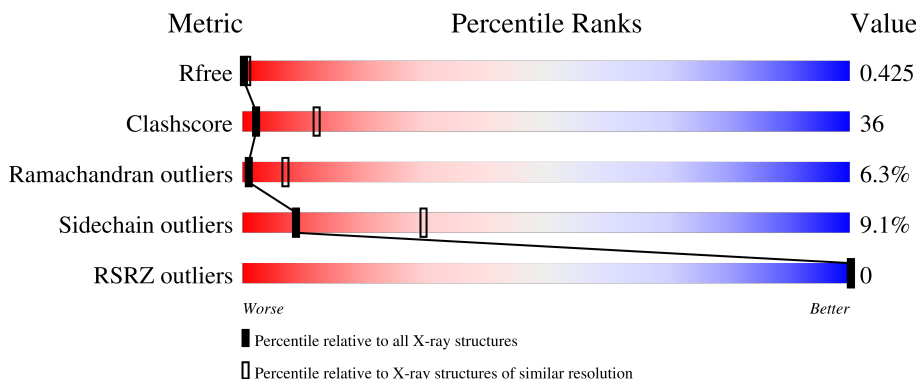
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

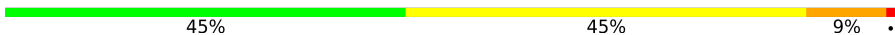
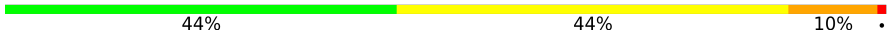
The reported resolution of this entry is 3.40 Å.

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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	525	
1	B	525	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8286 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4117	2634	671	794	18			
1	B	525	Total	C	N	O	S	0	0	0
			4117	2634	671	794	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	TYR	UNK	SEE REMARK 999	UNP Q9Q1V2
B	179	TYR	UNK	SEE REMARK 999	UNP Q9Q1V2

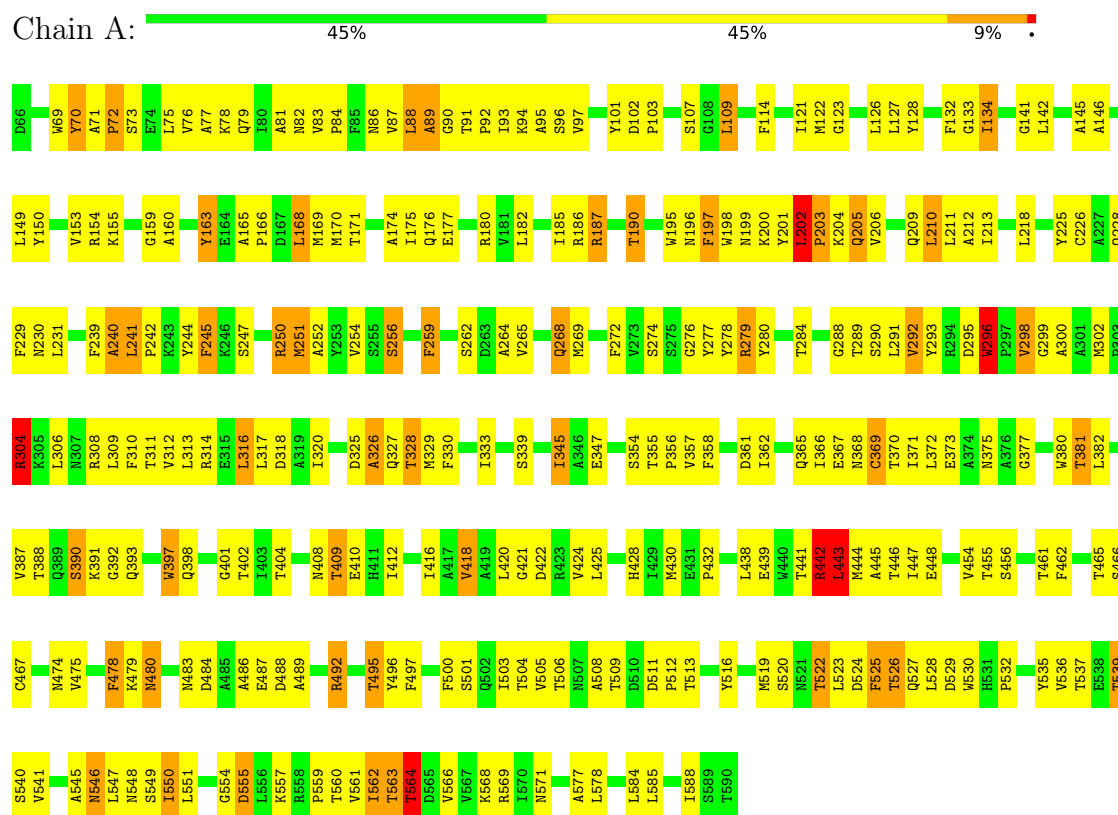
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	30	Total	O	0	0
			30	30		

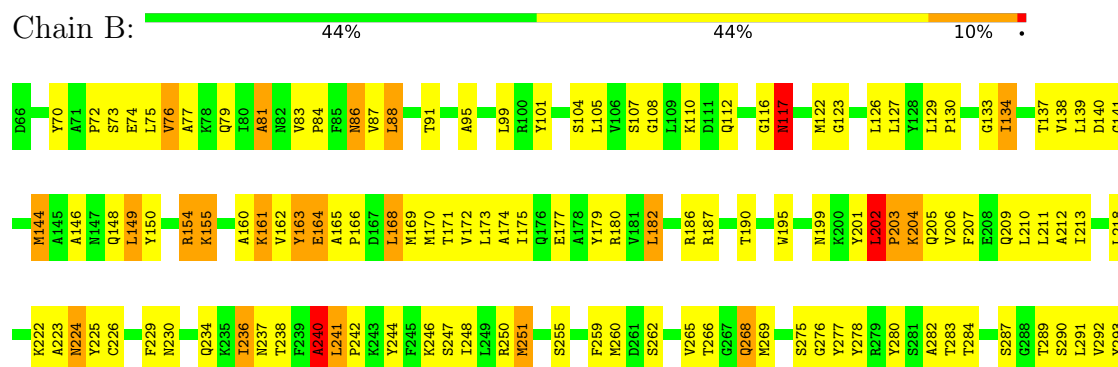
3 Residue-property plots

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



• Molecule 1: CAPSID PROTEIN



R294	E367	T446	T526
D295	N368	I447	Q527
V296	C369	V454	L528
P297	T370	V454	D529
V298	I371	S457	W530
Q299	L372	E458	I533
A300	E373	K459	I534
A301	A374	V460	Y535
M302	N375	T461	V536
P303	W380	F462	
R304	T381	T465	T539
K305	L382	S466	S540
L306		C467	V541
M307	N386	E470	R542
R308	T387	L471	N543
L309	Q388	V475	V544
V312	Q389	Y476	A545
	S390	Y477	N546
L316	K391	K478	L547
	G392	K479	N548
I320	Q393		S549
	V394	W482	T550
D323	L395		
A324	L396	A486	G554
D325	W397	E487	D555
A326	G401	D488	L556
Q327	N408	Q491	K557
T328	T409	R492	R558
M329	E410	V493	P559
F330	I412	F497	T560
I333	I416	S498	V561
	A417	S501	I562
G338	V418	Q502	T563
S339	A419	I503	T564
D340	L420	T504	
G341	D422	V505	K568
S344	R423	T506	R569
E347	V424	R507	I570
I348	L425	A508	N571
	M430	T509	S572
D351	Y434	D510	A577
E352	S435	P512	L578
T353	D436	T513	
S354	V437	S514	S581
T355	L438	A515	A582
P356	E439	M519	N583
V357	W440	S520	L584
D359	T441		L585
V360	R442		S586
D361	L443		N587
I362	M444		I588
L363	A445		S589
A364			T590
Q365			
I366			

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	407.42Å 407.42Å 808.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.98 – 3.40 49.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	70.0 (49.98-3.40) 43.5 (49.98-3.40)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.273 , 0.272 0.425 , 0.425	Depositor DCC
R_{free} test set	23009 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.087 for -h,-k,l	Xtriage
F_o, F_c correlation	0.19	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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	0.55	0/4209	1.06	21/5737 (0.4%)
1	B	0.57	1/4209 (0.0%)	1.08	21/5737 (0.4%)
All	All	0.56	1/8418 (0.0%)	1.07	42/11474 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	587	ASN	CA-C	5.28	1.58	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	TRP	CA-C-N	-11.14	105.91	119.84
1	A	296	TRP	C-N-CA	-11.14	105.91	119.84
1	B	296	TRP	CA-C-N	-10.17	107.13	119.84
1	B	296	TRP	C-N-CA	-10.17	107.13	119.84
1	B	304	ARG	N-CA-C	8.87	121.77	110.24

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	4117	0	4038	299	0
1	B	4117	0	4038	334	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	22	0	0	2	0
2	B	30	0	0	0	0
All	All	8286	0	8076	595	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 36.

The worst 5 of 595 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:B:72:PRO:HG2	1:B:76:VAL:HG11	1.34	1.05
1:B:419:ALA:HB1	1:B:447:ILE:HD13	1.40	1.03
1:A:187:ARG:HG2	1:A:187:ARG:HH11	1.26	0.99
1:A:442:ARG:N	1:A:442:ARG:HH11	1.62	0.97
1:A:381:THR:HG22	1:A:402:THR:H	1.30	0.96

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	523/525 (100%)	408 (78%)	84 (16%)	31 (6%)	1	8
1	B	523/525 (100%)	414 (79%)	74 (14%)	35 (7%)	1	6
All	All	1046/1050 (100%)	822 (79%)	158 (15%)	66 (6%)	1	7

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	202	LEU

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Mol	Chain	Res	Type
1	A	203	PRO
1	A	205	GLN
1	A	326	ALA

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	449/449 (100%)	407 (91%)	42 (9%)	8	29
1	B	449/449 (100%)	409 (91%)	40 (9%)	9	31
All	All	898/898 (100%)	816 (91%)	82 (9%)	9	30

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	283	THR
1	B	457	SER
1	B	295	ASP
1	B	388	THR
1	B	478	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	ASN
1	B	193	ASN
1	B	583	ASN
1	B	176	GLN
1	B	209	GLN

5.3.3 RNA ⓘ

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 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 [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	525/525 (100%)	-0.42	0 100 100	16, 31, 60, 85	0
1	B	525/525 (100%)	-0.44	0 100 100	14, 31, 62, 103	0
All	All	1050/1050 (100%)	-0.43	0 100 100	14, 31, 62, 103	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.