



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:15 AM UTC

PDB ID : 8UFO / pdb_00008ufo
Title : Crystal Structure of Gastrointestinal HAstV VA1 capsid spike domain at 1.46 Å resolution
Authors : Ghosh, A.; DuBois, R.M.
Deposited on : 2023-10-04
Resolution : 1.46 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

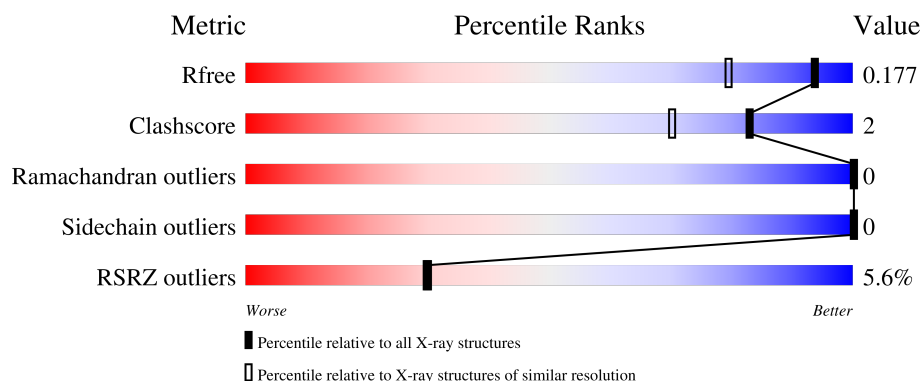
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	289	5% 89% 5% 6%
1	C	289	5% 87% 7% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4881 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 polypeptide VP90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	5	0
			2170	1382	374	403	11			
1	C	269	Total	C	N	O	S	0	4	0
			2152	1374	373	393	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	MET	-	initiating methionine	UNP C7BG48
A	407	GLY	-	expression tag	UNP C7BG48
A	420	PHE	TYR	conflict	UNP C7BG48
A	670	THR	SER	conflict	UNP C7BG48
A	685	ALA	-	expression tag	UNP C7BG48
A	686	ALA	-	expression tag	UNP C7BG48
A	687	ALA	-	expression tag	UNP C7BG48
A	688	GLU	-	expression tag	UNP C7BG48
A	689	LEU	-	expression tag	UNP C7BG48
A	690	ALA	-	expression tag	UNP C7BG48
A	691	LEU	-	expression tag	UNP C7BG48
A	692	VAL	-	expression tag	UNP C7BG48
A	693	PRO	-	expression tag	UNP C7BG48
A	694	ARG	-	expression tag	UNP C7BG48
C	406	MET	-	initiating methionine	UNP C7BG48
C	407	GLY	-	expression tag	UNP C7BG48
C	420	PHE	TYR	conflict	UNP C7BG48
C	670	THR	SER	conflict	UNP C7BG48
C	685	ALA	-	expression tag	UNP C7BG48
C	686	ALA	-	expression tag	UNP C7BG48
C	687	ALA	-	expression tag	UNP C7BG48
C	688	GLU	-	expression tag	UNP C7BG48
C	689	LEU	-	expression tag	UNP C7BG48
C	690	ALA	-	expression tag	UNP C7BG48
C	691	LEU	-	expression tag	UNP C7BG48

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Chain	Residue	Modelled	Actual	Comment	Reference
C	692	VAL	-	expression tag	UNP C7BG48
C	693	PRO	-	expression tag	UNP C7BG48
C	694	ARG	-	expression tag	UNP C7BG48

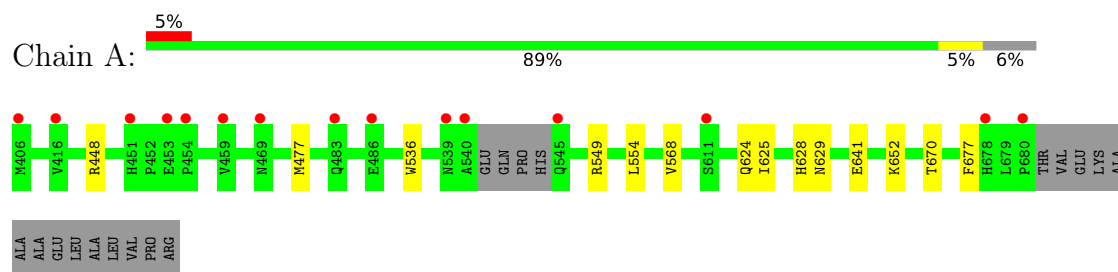
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	294	Total 294	O 294	0	0
2	C	265	Total 265	O 265	0	0

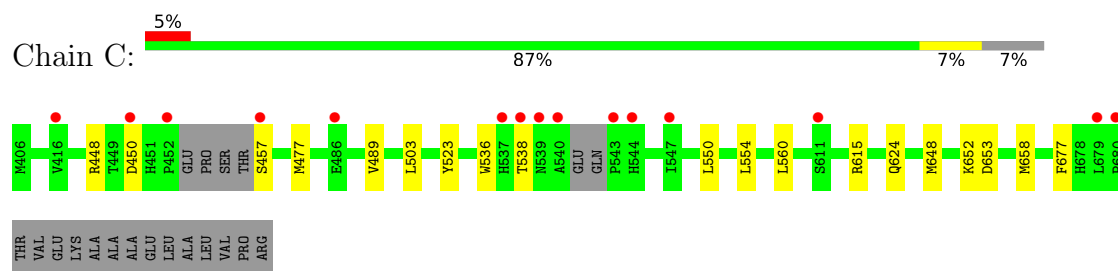
3 Residue-property plots [i](#)

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 polyprotein VP90



- Molecule 1: Capsid polyprotein VP90



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.62Å 82.56Å 61.12Å 90.00° 102.71° 90.00°	Depositor
Resolution (Å)	41.28 – 1.46 41.28 – 1.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.28-1.46) 99.5 (41.28-1.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.49 (at 1.46Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.153 , 0.177 0.153 , 0.177	Depositor DCC
R_{free} test set	2000 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4881	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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	0.30	0/2241	0.59	0/3059
1	C	0.32	0/2223	0.60	0/3030
All	All	0.31	0/4464	0.60	0/6089

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	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	448[A]	ARG	Sidechain
1	C	448[B]	ARG	Sidechain

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	2170	0	2103	10	0
1	C	2152	0	2091	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	294	0	0	2	0
2	C	265	0	0	1	0
All	All	4881	0	4194	20	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 2.

All (20) 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:C:450:ASP:OD1	2:C:701:HOH:O	2.07	0.72
1:C:550:LEU:HD21	1:C:658:MET:HB3	1.74	0.70
1:A:641:GLU:OE1	2:A:702:HOH:O	2.18	0.56
1:C:477[A]:MET:HG2	1:C:624:GLN:HA	1.88	0.56
1:C:477[A]:MET:HE3	1:C:624:GLN:HB2	1.90	0.54
1:A:629:ASN:ND2	2:A:704:HOH:O	2.37	0.52
1:A:477[A]:MET:HG2	1:A:624:GLN:HA	1.94	0.49
1:C:538:THR:HG22	1:C:648:MET:HE1	1.93	0.49
1:A:554:LEU:HB2	1:A:677:PHE:CE1	2.51	0.46
1:A:549[A]:ARG:HB2	1:A:628:HIS:CE1	2.51	0.45
1:C:489:VAL:HG21	1:C:503:LEU:HG	1.99	0.44
1:C:560:LEU:HD13	1:C:615:ARG:HG2	1.99	0.44
1:A:536:TRP:CE2	1:A:652:LYS:HB2	2.52	0.43
1:C:554:LEU:HB2	1:C:677:PHE:CE1	2.54	0.43
1:A:670:THR:HB	1:C:653:ASP:HA	2.01	0.42
1:A:477[A]:MET:HE3	1:A:624:GLN:HB2	2.01	0.42
1:C:457:SER:HB2	1:C:523:TYR:CE1	2.54	0.42
1:C:536:TRP:CE2	1:C:652:LYS:HB2	2.54	0.42
1:A:448[B]:ARG:HD2	1:A:568:VAL:HG21	2.00	0.41
1:A:477[B]:MET:HE1	1:A:625:ILE:HG22	2.03	0.41

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	272/289 (94%)	270 (99%)	2 (1%)	0	100	100
1	C	266/289 (92%)	263 (99%)	3 (1%)	0	100	100
All	All	538/578 (93%)	533 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	237/246 (96%)	237 (100%)	0	100	100
1	C	234/246 (95%)	234 (100%)	0	100	100
All	All	471/492 (96%)	471 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	A	527	ASN
1	A	537	HIS
1	A	558	ASN
1	A	590	GLN
1	A	609	GLN
1	A	651	GLN
1	C	584	GLN
1	C	651	GLN

5.3.3 RNA [i](#)

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 ⓘ

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	271/289 (93%)	-0.11	15 (5%)	30 30	3, 11, 26, 41	5 (1%)
1	C	269/289 (93%)	0.01	15 (5%)	30 30	6, 11, 30, 42	4 (1%)
All	All	540/578 (93%)	-0.05	30 (5%)	30 30	3, 11, 27, 42	9 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	679	LEU	6.0
1	C	680	PRO	4.4
1	C	486	GLU	4.3
1	C	543	PRO	4.1
1	A	611	SER	4.0
1	C	457	SER	3.5
1	C	547	ILE	3.5
1	A	680	PRO	3.3
1	C	611	SER	3.2
1	C	540	ALA	3.1
1	A	453	GLU	3.1
1	C	538	THR	3.0
1	C	450	ASP	2.8
1	A	540	ALA	2.8
1	C	416	VAL	2.7
1	C	539	ASN	2.7
1	A	483	GLN	2.6
1	A	486	GLU	2.6
1	A	459	VAL	2.6
1	A	451	HIS	2.5
1	A	469	ASN	2.5
1	C	544	HIS	2.5
1	A	539	ASN	2.5
1	C	452	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	416	VAL	2.3
1	A	406	MET	2.2
1	A	545	GLN	2.2
1	A	454	PRO	2.1
1	A	678	HIS	2.0
1	C	537	HIS	2.0

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.