



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:10 PM UTC

PDB ID : 4EJR / pdb\_00004ejr  
Title : Crystal structure of major capsid protein S domain from rabbit hemorrhagic disease virus  
Authors : Xu, F.; Ma, J.; Zhang, K.; Wang, X.; Sun, F.  
Deposited on : 2012-04-07  
Resolution : 2.00 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

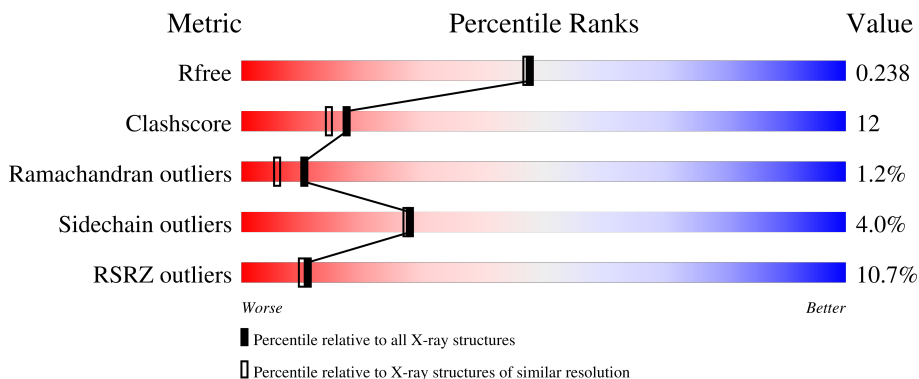
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 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	255	
1	B	255	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2598 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 Major capsid protein VP60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	163	1260	815	211	229	5	0	0	0
1	B	163	1260	815	211	229	5	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP Q3HNQ1
A	-23	GLY	-	expression tag	UNP Q3HNQ1
A	-22	HIS	-	expression tag	UNP Q3HNQ1
A	-21	HIS	-	expression tag	UNP Q3HNQ1
A	-20	HIS	-	expression tag	UNP Q3HNQ1
A	-19	HIS	-	expression tag	UNP Q3HNQ1
A	-18	HIS	-	expression tag	UNP Q3HNQ1
A	-17	HIS	-	expression tag	UNP Q3HNQ1
A	-16	HIS	-	expression tag	UNP Q3HNQ1
A	-15	HIS	-	expression tag	UNP Q3HNQ1
A	-14	SER	-	expression tag	UNP Q3HNQ1
A	-13	SER	-	expression tag	UNP Q3HNQ1
A	-12	GLY	-	expression tag	UNP Q3HNQ1
A	-11	GLU	-	expression tag	UNP Q3HNQ1
A	-10	ASN	-	expression tag	UNP Q3HNQ1
A	-9	LEU	-	expression tag	UNP Q3HNQ1
A	-8	TYR	-	expression tag	UNP Q3HNQ1
A	-7	PHE	-	expression tag	UNP Q3HNQ1
A	-6	GLN	-	expression tag	UNP Q3HNQ1
A	-5	GLY	-	expression tag	UNP Q3HNQ1
A	-4	SER	-	expression tag	UNP Q3HNQ1
A	-3	LYS	-	expression tag	UNP Q3HNQ1
A	-2	LEU	-	expression tag	UNP Q3HNQ1
A	-1	GLU	-	expression tag	UNP Q3HNQ1
A	0	PHE	-	expression tag	UNP Q3HNQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	expression tag	UNP Q3HNQ1
B	-23	GLY	-	expression tag	UNP Q3HNQ1
B	-22	HIS	-	expression tag	UNP Q3HNQ1
B	-21	HIS	-	expression tag	UNP Q3HNQ1
B	-20	HIS	-	expression tag	UNP Q3HNQ1
B	-19	HIS	-	expression tag	UNP Q3HNQ1
B	-18	HIS	-	expression tag	UNP Q3HNQ1
B	-17	HIS	-	expression tag	UNP Q3HNQ1
B	-16	HIS	-	expression tag	UNP Q3HNQ1
B	-15	HIS	-	expression tag	UNP Q3HNQ1
B	-14	SER	-	expression tag	UNP Q3HNQ1
B	-13	SER	-	expression tag	UNP Q3HNQ1
B	-12	GLY	-	expression tag	UNP Q3HNQ1
B	-11	GLU	-	expression tag	UNP Q3HNQ1
B	-10	ASN	-	expression tag	UNP Q3HNQ1
B	-9	LEU	-	expression tag	UNP Q3HNQ1
B	-8	TYR	-	expression tag	UNP Q3HNQ1
B	-7	PHE	-	expression tag	UNP Q3HNQ1
B	-6	GLN	-	expression tag	UNP Q3HNQ1
B	-5	GLY	-	expression tag	UNP Q3HNQ1
B	-4	SER	-	expression tag	UNP Q3HNQ1
B	-3	LYS	-	expression tag	UNP Q3HNQ1
B	-2	LEU	-	expression tag	UNP Q3HNQ1
B	-1	GLU	-	expression tag	UNP Q3HNQ1
B	0	PHE	-	expression tag	UNP Q3HNQ1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	30	Total O 30 30	0	0
2	B	48	Total O 48 48	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.73Å 48.36Å 65.16Å 90.00° 100.95° 90.00°	Depositor
Resolution (Å)	49.35 – 2.00 49.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.35-2.00) 99.7 (49.35-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.201 , 0.241 0.201 , 0.238	Depositor DCC
$R_{free}$ test set	1330 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5598e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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	1.41	4/1300 (0.3%)	1.23	6/1785 (0.3%)
1	B	1.53	10/1300 (0.8%)	1.26	9/1785 (0.5%)
All	All	1.47	14/2600 (0.5%)	1.24	15/3570 (0.4%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	ASP	N-CA	6.44	1.54	1.46
1	B	128	VAL	N-CA	6.41	1.51	1.46
1	B	211	VAL	CA-CB	5.94	1.61	1.54
1	A	104	ALA	CA-CB	5.92	1.62	1.53
1	B	89	ILE	CA-CB	5.78	1.60	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ILE	CB-CA-C	-7.36	100.48	110.42
1	B	203	GLY	CA-C-N	-6.14	115.03	121.35
1	B	203	GLY	C-N-CA	-6.14	115.03	121.35
1	A	176	ASN	N-CA-C	6.12	120.35	113.01
1	A	100	ASN	CA-C-N	-5.91	113.59	119.56

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	1260	0	1226	25	0
1	B	1260	0	1226	42	0
2	A	30	0	0	0	0
2	B	48	0	0	0	0
All	All	2598	0	2452	62	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 12.

The worst 5 of 62 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:145:GLY:HA2	1:B:148:LEU:CD2	1.49	1.39
1:B:145:GLY:CA	1:B:148:LEU:HD23	1.80	1.11
1:B:145:GLY:CA	1:B:148:LEU:CD2	2.29	1.09
1:B:145:GLY:C	1:B:148:LEU:HD23	1.81	1.04
1:B:145:GLY:HA2	1:B:148:LEU:HD23	1.31	1.04

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	161/255 (63%)	154 (96%)	6 (4%)	1 (1%)	21 17
1	B	161/255 (63%)	153 (95%)	5 (3%)	3 (2%)	6 3
All	All	322/510 (63%)	307 (95%)	11 (3%)	4 (1%)	10 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	SER

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Mol	Chain	Res	Type
1	B	145	GLY
1	B	146	PRO
1	A	204	GLY

### 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	137/206 (66%)	129 (94%)	8 (6%)	18	15
1	B	137/206 (66%)	134 (98%)	3 (2%)	45	50
All	All	274/412 (66%)	263 (96%)	11 (4%)	28	27

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	PHE
1	B	81	SER
1	B	177	MET
1	B	148	LEU
1	A	174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	GLN
1	B	152	GLN
1	B	210	GLN
1	B	196	ASN
1	A	196	ASN

### 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	163/255 (63%)	0.31	23 (14%) <b>6</b> <b>5</b>	13, 21, 53, 62	0
1	B	163/255 (63%)	0.02	12 (7%) <b>20</b> <b>19</b>	11, 19, 40, 53	0
All	All	326/510 (63%)	0.16	35 (10%) <b>11</b> <b>10</b>	11, 20, 48, 62	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	PRO	5.5
1	A	146	PRO	5.0
1	A	148	LEU	4.8
1	B	203	GLY	4.7
1	A	202	PHE	4.2

### 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.