



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:33 PM UTC

PDB ID : 1VHI / pdb_00001vhi
Title : EPSTEIN BARR VIRUS NUCLEAR ANTIGEN-1 DNA-BINDING DOMAIN, RESIDUES 470-607
Authors : Bochkarev, A.; Barwell, J.; Pfuetzner, R.; Furey, W.; Edwards, A.; Frappier, L.
Deposited on : 1996-10-05
Resolution : 2.50 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

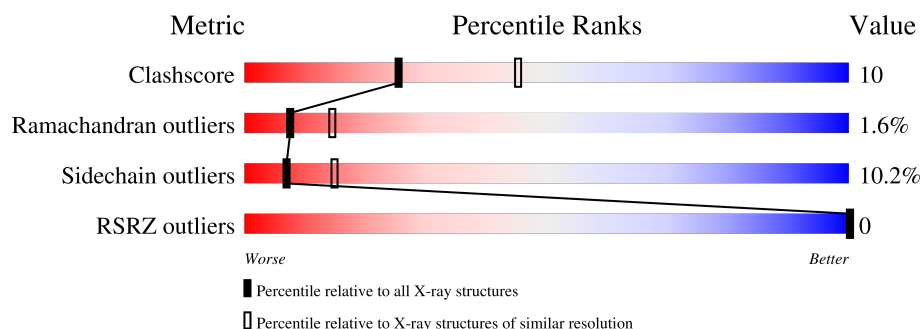
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	142	
1	B	142	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2727 atoms, of which 585 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 EPSTEIN BARR VIRUS NUCLEAR ANTIGEN-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	139	Total	C	H	N	O	S	0	0	0
			1284	673	227	184	192	8			
1	B	132	Total	C	H	N	O	S	0	0	0
			1230	650	216	175	182	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	SER	LYS	conflict	UNP P03211
A	469	MET	ARG	conflict	UNP P03211
B	467	SER	LYS	conflict	UNP P03211
B	469	MET	ARG	conflict	UNP P03211

- Molecule 2 is water.

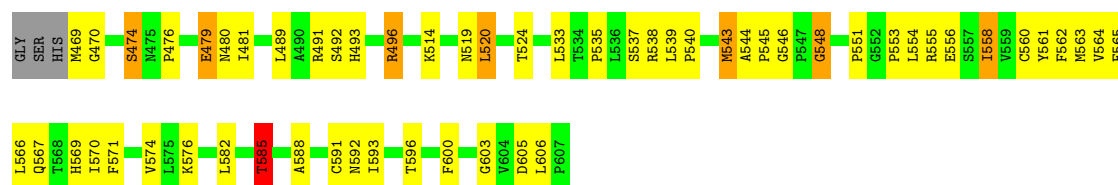
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	38	Total	H	O	0	0
			114	76	38		
2	B	33	Total	H	O	0	0
			99	66	33		

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.

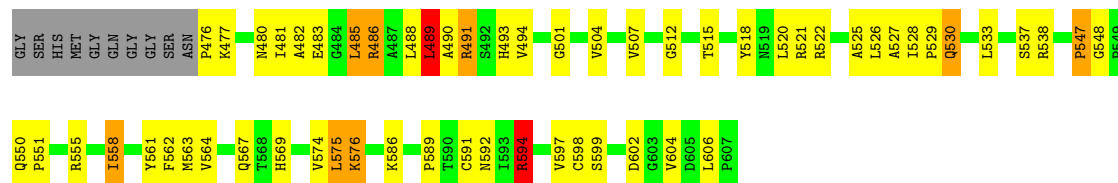
• Molecule 1: EPSTEIN BARR VIRUS NUCLEAR ANTIGEN-1

Chain A: 



• Molecule 1: EPSTEIN BARR VIRUS NUCLEAR ANTIGEN-1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.99Å 69.08Å 70.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (8.00-2.50) 92.1 (8.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.179 , (Not available) 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2727	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 15.03% 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

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	1.20	2/1082 (0.2%)	1.97	26/1469 (1.8%)
1	B	1.18	2/1039 (0.2%)	2.05	32/1412 (2.3%)
All	All	1.19	4/2121 (0.2%)	2.01	58/2881 (2.0%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	493	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	493	HIS	CD2-NE2	-5.40	1.31	1.37
1	B	569	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	569	HIS	CD2-NE2	-5.11	1.32	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	MET	N-CA-C	9.68	121.83	111.28
1	A	562	PHE	CA-CB-CG	8.79	122.59	113.80
1	A	567	GLN	OE1-CD-NE2	-8.51	114.09	122.60
1	B	493	HIS	N-CA-C	-8.18	94.92	108.34
1	B	480	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	B	551	PRO	N-CA-C	7.86	125.47	113.75
1	A	543	MET	CA-C-N	-7.86	114.41	122.74
1	A	543	MET	C-N-CA	-7.86	114.41	122.74
1	A	585	THR	N-CA-CB	-7.77	97.35	110.41
1	A	570	ILE	CA-C-O	-7.62	112.56	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	515	THR	N-CA-CB	-7.50	97.82	110.49
1	B	592	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	A	592	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	B	562	PHE	CA-CB-CG	6.80	120.60	113.80
1	B	489	LEU	N-CA-C	-6.67	103.93	111.14
1	A	543	MET	CG-SD-CE	-6.66	86.24	100.90
1	B	507	VAL	N-CA-C	-6.63	98.83	108.11
1	A	519	ASN	OD1-CG-ND2	-6.53	116.08	122.60
1	B	550	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	B	558	ILE	CB-CG1-CD1	-6.38	100.40	113.80
1	A	596	THR	CA-CB-OG1	-6.34	100.09	109.60
1	B	574	VAL	N-CA-CB	-6.32	102.48	110.57
1	B	592	ASN	CB-CG-ND2	5.94	125.31	116.40
1	A	479	GLU	CB-CG-CD	5.90	122.63	112.60
1	B	485	LEU	O-C-N	5.87	128.11	122.07
1	A	481	ILE	N-CA-C	-5.74	105.13	110.53
1	A	543	MET	CA-CB-CG	-5.74	102.62	114.10
1	B	602	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	530	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	603	GLY	O-C-N	-5.71	116.65	122.70
1	B	512	GLY	CA-C-O	-5.68	114.62	121.67
1	B	481	ILE	CA-C-O	-5.67	115.16	121.05
1	B	564	VAL	N-CA-C	-5.66	99.48	107.75
1	A	524	THR	N-CA-C	-5.61	104.38	111.11
1	A	606	LEU	CA-C-O	-5.60	114.52	120.23
1	B	558	ILE	N-CA-C	-5.52	107.37	112.83
1	A	469	MET	CG-SD-CE	5.51	113.03	100.90
1	A	545	PRO	N-CA-C	-5.51	102.54	111.14
1	B	480	ASN	N-CA-C	-5.51	104.91	111.03
1	B	525	ALA	N-CA-C	5.49	117.35	111.36
1	A	548	GLY	N-CA-C	5.36	123.27	112.34
1	A	480	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	B	589	PRO	N-CD-CG	-5.32	97.42	103.80
1	B	476	PRO	N-CA-CB	5.30	108.83	103.00
1	B	491	ARG	CA-CB-CG	5.29	124.69	114.10
1	B	501	GLY	N-CA-C	-5.27	107.99	115.43
1	B	558	ILE	N-CA-CB	-5.21	103.34	112.08
1	A	570	ILE	N-CA-C	-5.16	105.37	111.00
1	B	493	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	B	594	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	B	512	GLY	O-C-N	-5.08	116.98	122.62
1	A	493	HIS	CB-CG-CD2	-5.07	124.61	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	PHE	N-CA-C	-5.07	101.44	109.76
1	B	550	GLN	CG-CD-NE2	5.04	123.97	116.40
1	A	481	ILE	CA-CB-CG1	-5.04	101.84	110.40
1	A	546	GLY	N-CA-C	5.03	122.59	112.34
1	B	575	LEU	O-C-N	-5.02	116.42	122.15
1	B	527	ALA	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	594	ARG	Sidechain

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	1057	227	1067	19	1
1	B	1014	216	1031	22	0
2	A	38	76	0	1	0
2	B	33	66	0	1	0
All	All	2142	585	2098	40	1

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 10.

All (40) 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:594:ARG:HH11	1:B:594:ARG:HB3	1.51	0.76
1:A:476:PRO:HG2	1:A:479:GLU:HB2	1.73	0.69
1:A:520:LEU:HD12	1:A:593:ILE:HD13	1.74	0.69
1:A:538:ARG:HH21	1:A:558:ILE:HG22	1.60	0.66
1:A:551:PRO:HG2	1:A:554:LEU:HD12	1.82	0.61
1:B:538:ARG:HH21	1:B:558:ILE:HD12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:MET:HE1	1:B:598:CYS:SG	2.41	0.60
1:B:488:LEU:O	1:B:491:ARG:HG2	2.04	0.57
1:A:582:LEU:O	1:A:585:THR:HB	2.06	0.56
1:A:571:PHE:HA	1:A:574:VAL:HG22	1.93	0.51
1:B:537:SER:HB3	1:B:561:TYR:CE2	2.47	0.50
1:B:563:MET:HE2	1:B:563:MET:HB3	1.70	0.49
1:B:529:PRO:HD2	1:B:530:GLN:OE1	2.14	0.48
1:B:518:TYR:O	1:B:522:ARG:HG2	2.14	0.47
1:B:485:LEU:O	1:B:489:LEU:HB2	2.14	0.47
1:B:528:ILE:HD11	1:B:575:LEU:HD13	1.96	0.46
1:B:586:LYS:O	1:B:591:CYS:HB3	2.14	0.46
1:A:537:SER:HB3	1:A:561:TYR:CE1	2.50	0.46
1:A:540:PRO:HA	1:A:556:GLU:HA	1.98	0.45
1:A:588:ALA:HA	1:A:591:CYS:SG	2.57	0.45
1:B:538:ARG:NH2	1:B:558:ILE:HD12	2.32	0.44
1:B:576:LYS:HE2	1:B:576:LYS:HB3	1.81	0.44
1:B:604:VAL:HG12	1:B:606:LEU:HD12	1.98	0.44
1:B:538:ARG:HG3	1:B:538:ARG:HH11	1.83	0.44
1:B:522:ARG:O	1:B:526:LEU:HD13	2.17	0.43
1:B:567:GLN:HG3	2:B:13:HOH:O	2.18	0.43
1:A:496:ARG:HD3	2:A:46:HOH:O	2.18	0.43
1:A:588:ALA:N	1:A:591:CYS:SG	2.92	0.43
1:A:548:GLY:HA3	1:A:555:ARG:NE	2.34	0.42
1:A:470:GLY:HA3	1:A:474:SER:O	2.20	0.42
1:B:521:ARG:HG3	1:B:533:LEU:HD22	2.01	0.42
1:B:482:ALA:O	1:B:486:ARG:HB2	2.20	0.42
1:A:548:GLY:HA3	1:A:555:ARG:CZ	2.50	0.42
1:B:538:ARG:HG3	1:B:538:ARG:NH1	2.35	0.41
1:A:514:LYS:HD2	1:A:560:CYS:SG	2.61	0.41
1:A:563:MET:HE1	1:A:600:PHE:HZ	1.86	0.41
1:A:605:ASP:OD2	1:B:594:ARG:NH2	2.54	0.41
1:B:576:LYS:HG3	1:B:597:VAL:HG23	2.03	0.41
1:A:539:LEU:HD13	1:A:561:TYR:CD1	2.56	0.41
1:A:533:LEU:HD23	1:A:564:VAL:HG22	2.02	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HH22	1:A:544:ALA:H[3_544]	1.30	0.30

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	114/142 (80%)	108 (95%)	5 (4%)	1 (1%)	14	27
1	B	130/142 (92%)	121 (93%)	6 (5%)	3 (2%)	5	8
All	All	244/284 (86%)	229 (94%)	11 (4%)	4 (2%)	7	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	547	PRO
1	B	548	GLY
1	A	535	PRO
1	B	490	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	115/117 (98%)	104 (90%)	11 (10%)	8	17
1	B	111/117 (95%)	99 (89%)	12 (11%)	6	13
All	All	226/234 (97%)	203 (90%)	23 (10%)	7	15

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	SER
1	A	489	LEU

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Mol	Chain	Res	Type
1	A	492	SER
1	A	496	ARG
1	A	520	LEU
1	A	543	MET
1	A	553	PRO
1	A	558	ILE
1	A	566	LEU
1	A	576	LYS
1	A	585	THR
1	B	477	LYS
1	B	483	GLU
1	B	486	ARG
1	B	489	LEU
1	B	494	VAL
1	B	504	VAL
1	B	520	LEU
1	B	547	PRO
1	B	555	ARG
1	B	576	LYS
1	B	594	ARG
1	B	599	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	569	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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 [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	139/142 (97%)	-0.74	0 100 100	5, 12, 26, 39	0
1	B	132/142 (92%)	-0.67	0 100 100	5, 13, 28, 36	0
All	All	271/284 (95%)	-0.71	0 100 100	5, 12, 28, 39	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.