



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:31 PM UTC

PDB ID : 1VSF / pdb_00001vsf
Title : ASV INTEGRASE CORE DOMAIN WITH MN(II) COFACTOR AND
HEPES LIGAND, HIGH MG CONCENTRATION FORM
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Deposited on : 1995-11-29
Resolution : 2.05 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

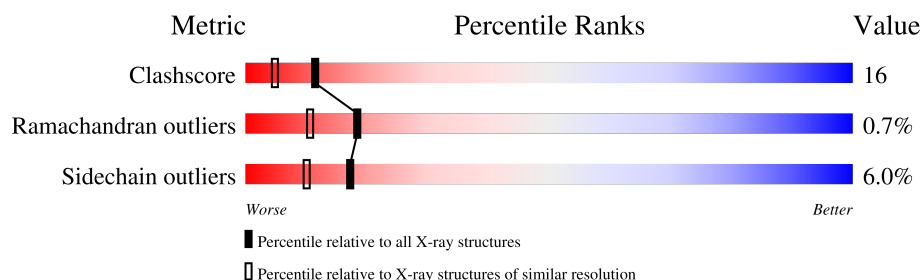
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	152	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1281 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 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1124	709	210	200	5			

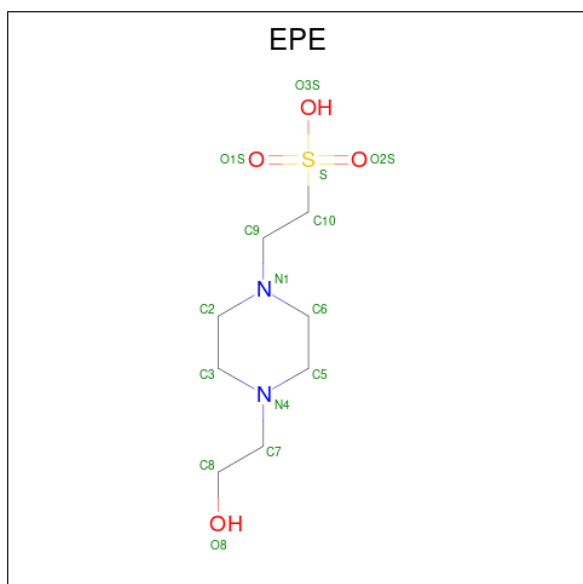
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ALA	VAL	conflict	UNP P03354
A	166	LYS	ARG	conflict	UNP P03354

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		

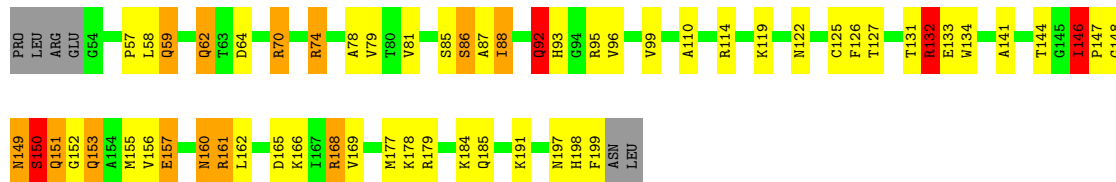
3 Residue-property plots [i](#)

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. 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. 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: INTEGRASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.24Å 66.24Å 81.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.05	Depositor
% Data completeness (in resolution range)	86.0 (8.00-2.05)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.130 , 0.189	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1281	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, MN

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	0.89	0/1149	2.41	74/1558 (4.7%)

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	A	0	2

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLN	CA-C-O	10.41	131.35	121.67
1	A	179	ARG	NE-CZ-NH2	-9.38	110.76	119.20
1	A	114	ARG	CD-NE-CZ	-9.38	111.28	124.40
1	A	132	ARG	NE-CZ-NH1	8.67	130.17	121.50
1	A	134	TRP	O-C-N	-8.55	113.05	122.12
1	A	96	VAL	CB-CA-C	8.51	123.47	111.81
1	A	126	PHE	CA-C-O	8.29	128.26	119.14
1	A	199	PHE	CA-CB-CG	-7.96	105.84	113.80
1	A	74	ARG	NE-CZ-NH2	-7.82	112.17	119.20
1	A	96	VAL	N-CA-CB	-7.80	102.24	111.60
1	A	146	ILE	N-CA-CB	7.78	118.00	109.99
1	A	59	GLN	OE1-CD-NE2	7.60	130.20	122.60
1	A	64	ASP	CA-C-O	-7.49	113.44	121.38
1	A	148	GLY	N-CA-C	-7.48	100.93	114.46
1	A	144	THR	N-CA-C	-7.32	103.66	112.59
1	A	197	ASN	CA-CB-CG	-7.05	105.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	LYS	CA-C-O	7.03	128.00	120.55
1	A	179	ARG	CA-C-O	-6.85	113.49	121.16
1	A	179	ARG	NE-CZ-NH1	6.68	128.19	121.50
1	A	70	ARG	CD-NE-CZ	-6.65	115.09	124.40
1	A	127	THR	CA-C-O	-6.56	111.52	119.32
1	A	132	ARG	CA-CB-CG	-6.51	101.08	114.10
1	A	132	ARG	CD-NE-CZ	6.50	133.50	124.40
1	A	148	GLY	CA-C-O	6.50	127.48	119.88
1	A	93	HIS	CA-C-N	6.45	128.47	120.34
1	A	93	HIS	C-N-CA	6.45	128.47	120.34
1	A	149	ASN	CA-C-O	6.40	127.24	119.49
1	A	166	LYS	O-C-N	-6.31	115.43	122.12
1	A	197	ASN	CB-CA-C	-6.24	98.32	109.24
1	A	74	ARG	CA-C-O	6.21	130.83	122.51
1	A	157	GLU	CA-C-O	6.18	126.97	120.42
1	A	191	LYS	CA-C-O	-6.04	114.02	120.42
1	A	160	ASN	N-CA-CB	6.00	119.04	110.16
1	A	184	LYS	O-C-N	-5.94	114.63	122.42
1	A	58	LEU	N-CA-C	-5.87	101.79	110.48
1	A	62	GLN	CA-C-O	-5.82	114.08	120.36
1	A	134	TRP	CA-C-N	5.79	128.51	120.29
1	A	134	TRP	C-N-CA	5.79	128.51	120.29
1	A	114	ARG	CB-CG-CD	-5.74	98.10	111.30
1	A	149	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	62	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	148	GLY	CA-C-N	5.67	129.68	120.60
1	A	148	GLY	C-N-CA	5.67	129.68	120.60
1	A	185	GLN	O-C-N	5.61	127.85	122.07
1	A	168	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	A	184	LYS	CA-C-N	5.57	127.68	120.44
1	A	184	LYS	C-N-CA	5.57	127.68	120.44
1	A	92	GLN	N-CA-CB	-5.54	101.99	110.85
1	A	153	GLN	CB-CG-CD	-5.52	103.21	112.60
1	A	141	ALA	CA-C-O	5.49	127.31	121.05
1	A	126	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	57	PRO	CA-C-O	5.46	127.89	121.56
1	A	177	MET	CA-C-O	-5.44	112.71	119.18
1	A	122	ASN	CA-CB-CG	-5.42	107.17	112.60
1	A	153	GLN	OE1-CD-NE2	5.42	128.02	122.60
1	A	169	VAL	N-CA-CB	-5.39	103.21	110.54
1	A	198	HIS	N-CA-C	5.35	117.68	109.07
1	A	132	ARG	NE-CZ-NH2	-5.34	114.40	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ALA	CA-C-O	5.33	126.12	120.10
1	A	153	GLN	CG-CD-NE2	-5.32	108.42	116.40
1	A	198	HIS	O-C-N	5.31	129.55	123.29
1	A	131	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	153	GLN	N-CA-C	5.22	117.92	109.83
1	A	78	ALA	O-C-N	-5.20	117.40	123.27
1	A	88	ILE	CB-CA-C	-5.19	102.89	110.62
1	A	95	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	162	LEU	CA-C-O	5.18	126.04	120.55
1	A	78	ALA	N-CA-C	-5.13	100.87	109.24
1	A	146	ILE	CB-CA-C	-5.07	106.03	111.00
1	A	184	LYS	CA-C-O	5.02	124.88	119.15
1	A	133	GLU	CB-CG-CD	5.01	121.12	112.60
1	A	95	ARG	CA-C-N	-5.01	116.74	122.95
1	A	95	ARG	C-N-CA	-5.01	116.74	122.95
1	A	150	SER	N-CA-C	-5.01	105.89	113.51

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Sidechain
1	A	70	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	1124	0	1139	37	0
2	A	1	0	0	0	0
3	A	15	0	18	0	0
4	A	141	0	0	5	0
All	All	1281	0	1157	37	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 16.

All (37) 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:A:146:ILE:O	1:A:149:ASN:HB2	1.65	0.94
1:A:151:GLN:OE1	1:A:153:GLN:HG2	1.68	0.93
1:A:132:ARG:HD2	4:A:371:HOH:O	1.72	0.89
1:A:146:ILE:HB	1:A:149:ASN:HD22	1.40	0.85
1:A:146:ILE:HG23	1:A:147:PRO:HD2	1.66	0.76
1:A:161:ARG:CZ	1:A:165:ASP:HB2	2.19	0.73
1:A:151:GLN:NE2	1:A:157:GLU:OE2	2.21	0.72
1:A:151:GLN:CD	1:A:153:GLN:HG2	2.19	0.68
1:A:151:GLN:HG2	1:A:157:GLU:OE2	1.95	0.66
1:A:59:GLN:HB3	4:A:395:HOH:O	1.98	0.63
1:A:99:VAL:HG23	4:A:417:HOH:O	1.99	0.63
1:A:151:GLN:HG3	1:A:153:GLN:H	1.64	0.62
1:A:150:SER:O	1:A:151:GLN:CB	2.49	0.60
1:A:146:ILE:HB	1:A:149:ASN:ND2	2.14	0.59
1:A:81:VAL:HG22	1:A:88:ILE:HD12	1.84	0.59
1:A:150:SER:O	1:A:151:GLN:HB2	2.02	0.58
1:A:87:ALA:C	1:A:88:ILE:HD13	2.29	0.57
1:A:149:ASN:OD1	1:A:152:GLY:N	2.40	0.54
1:A:74:ARG:O	1:A:92:GLN:HG2	2.11	0.50
1:A:146:ILE:CG2	1:A:147:PRO:HD2	2.40	0.50
1:A:161:ARG:O	1:A:161:ARG:NE	2.44	0.50
1:A:161:ARG:NH2	1:A:165:ASP:CA	2.75	0.50
1:A:81:VAL:HG22	1:A:88:ILE:CD1	2.44	0.48
1:A:151:GLN:NE2	4:A:392:HOH:O	2.47	0.47
1:A:85:SER:O	1:A:86:SER:CB	2.61	0.47
1:A:88:ILE:HD13	1:A:88:ILE:N	2.30	0.47
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.81	0.45
1:A:81:VAL:HG11	1:A:155:MET:HE2	1.99	0.45
1:A:161:ARG:NH2	1:A:165:ASP:HB2	2.31	0.45
1:A:62:GLN:NE2	1:A:156:VAL:H	2.15	0.45
1:A:79:VAL:HG21	1:A:160:ASN:HD22	1.84	0.43
1:A:161:ARG:NH2	1:A:165:ASP:HA	2.34	0.42
1:A:125:CYS:SG	4:A:398:HOH:O	2.52	0.42
1:A:149:ASN:C	1:A:151:GLN:H	2.27	0.42
1:A:79:VAL:HG21	1:A:160:ASN:ND2	2.36	0.40
1:A:87:ALA:O	1:A:88:ILE:HD13	2.21	0.40
1:A:119:LYS:HD2	1:A:153:GLN:HB3	2.03	0.40

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	144/152 (95%)	138 (96%)	5 (4%)	1 (1%)	18	10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLN

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	116/122 (95%)	109 (94%)	7 (6%)	17	10

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	92	GLN
1	A	132	ARG
1	A	146	ILE
1	A	150	SER
1	A	161	ARG
1	A	178	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	92	GLN
1	A	160	ASN
1	A	185	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EPE	A	261	-	15,15,15	1.52	2 (13%)	19,20,20	1.61	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	261	-	-	0/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	261	EPE	O3S-S	4.41	1.63	1.47
3	A	261	EPE	C10-S	2.57	1.81	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	261	EPE	O2S-S-C10	4.75	113.90	106.73
3	A	261	EPE	C3-C2-N1	2.75	116.19	110.65
3	A	261	EPE	C5-C6-N1	-2.13	106.35	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.