



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:02 AM UTC

PDB ID : 1VSD / pdb_00001vsd
Title : ASV INTEGRASE CORE DOMAIN WITH MG(II) COFACTOR AND
HEPES LIGAND, HIGH MG CONCENTRATION FORM
Authors : Bujacz, G.; Jaskolski, M.; Alexandratos, J.; Wlodawer, A.
Deposited on : 1995-11-29
Resolution : 1.70 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

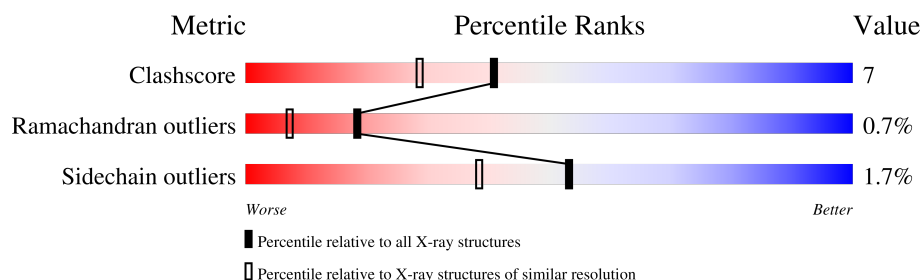
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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

There are 4 unique types of molecules in this entry. The entry contains 1316 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
			1127	711	210	201	5			

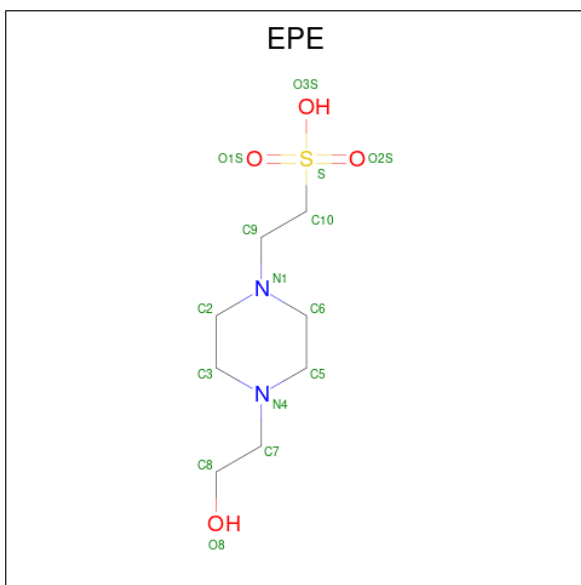
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	LEU	ALA	conflict	UNP P03354
A	52	ARG	LEU	conflict	UNP P03354
A	?	-	ALA	deletion	UNP P03354
A	?	-	GLY	deletion	UNP P03354
A	?	-	VAL	deletion	UNP P03354
A	?	-	ASN	deletion	UNP P03354
A	?	-	PRO	deletion	UNP P03354
A	?	-	ARG	deletion	UNP P03354
A	101	ALA	VAL	conflict	UNP P03354
A	166	LYS	ARG	conflict	UNP P03354

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	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.

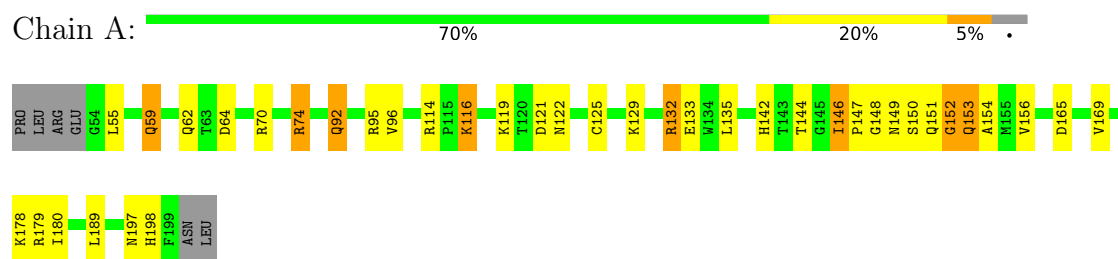
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		

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



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	66.05 Å 66.05 Å 81.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70	Depositor
% Data completeness (in resolution range)	91.6 (8.00-1.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.150 , 0.191	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1316	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: MG, EPE, OCY

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	0.88	0/1142	1.89	32/1547 (2.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	NE-CZ-NH2	-10.86	109.43	119.20
1	A	146	ILE	N-CA-CB	9.41	118.83	110.08
1	A	74	ARG	CD-NE-CZ	-8.14	113.00	124.40
1	A	178	LYS	CB-CA-C	-7.93	104.97	116.54
1	A	70	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	A	152	GLY	N-CA-C	-7.51	105.54	114.48
1	A	92	GLN	OE1-CD-NE2	7.46	130.06	122.60
1	A	153	GLN	OE1-CD-NE2	7.29	129.89	122.60
1	A	198	HIS	O-C-N	7.18	131.74	123.27
1	A	144	THR	N-CA-C	-6.70	104.23	112.88
1	A	132	ARG	CD-NE-CZ	6.28	133.19	124.40
1	A	62	GLN	CA-C-O	-6.17	114.04	120.70
1	A	92	GLN	CB-CA-C	-6.14	98.14	109.37
1	A	122	ASN	CA-CB-CG	-6.09	106.50	112.60
1	A	179	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	A	92	GLN	CG-CD-NE2	-6.08	107.28	116.40
1	A	59	GLN	CB-CG-CD	-6.06	102.29	112.60
1	A	153	GLN	CA-C-O	5.91	127.34	121.20
1	A	121	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	55	LEU	N-CA-C	-5.81	105.52	113.30
1	A	154	ALA	N-CA-C	-5.74	105.16	111.82
1	A	55	LEU	CA-C-O	5.70	126.10	119.32
1	A	133	GLU	CB-CG-CD	5.52	121.99	112.60
1	A	180	ILE	CA-C-O	5.23	123.76	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	116	LYS	N-CA-C	-5.17	106.12	112.90
1	A	64	ASP	CA-C-O	-5.10	115.82	121.33
1	A	197	ASN	CB-CA-C	-5.09	101.16	109.56
1	A	197	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	70	ARG	NH1-CZ-NH2	5.06	125.88	119.30
1	A	132	ARG	CA-CB-CG	-5.06	103.98	114.10
1	A	114	ARG	N-CA-CB	-5.05	102.84	110.32

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	1127	0	1143	15	0
2	A	1	0	0	0	0
3	A	15	0	18	0	0
4	A	173	0	0	1	1
All	All	1316	0	1161	15	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 7.

All (15) 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:59:GLN:HB2	1:A:116:LYS:HG2	1.73	0.71
1:A:129:LYS:HD3	1:A:129:LYS:C	2.17	0.69
1:A:152:GLY:HA2	4:A:372:HOH:O	1.94	0.67
1:A:149:ASN:C	1:A:151:GLN:H	2.09	0.59
1:A:149:ASN:HB3	1:A:151:GLN:O	2.09	0.53
1:A:150:SER:C	1:A:151:GLN:HG3	2.37	0.49
1:A:153:GLN:HB2	1:A:156:VAL:HG12	1.95	0.48
1:A:74:ARG:HH11	1:A:74:ARG:HD3	1.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASP:O	1:A:169:VAL:HG13	2.17	0.44
1:A:135:LEU:HD13	1:A:142:HIS:HB2	2.00	0.44
1:A:150:SER:O	1:A:151:GLN:HG3	2.18	0.44
1:A:92:GLN:HG3	1:A:189:LEU:HD22	2.01	0.43
1:A:149:ASN:O	1:A:150:SER:HB3	2.19	0.42
1:A:119:LYS:HB2	1:A:119:LYS:HE3	1.88	0.42
1:A:146:ILE:O	1:A:148:GLY:N	2.54	0.41

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)
4:A:282:HOH:O	4:A:418:HOH:O[7_556]	2.15	0.05

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	143/152 (94%)	137 (96%)	5 (4%)	1 (1%)	18 7

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO

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	115/121 (95%)	113 (98%)	2 (2%)	53 38

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	132	ARG

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

Mol	Chain	Res	Type
1	A	59	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	OCY	A	125	1	7,8,9	0.52	0	4,8,10	2.22	1 (25%)

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
1	OCY	A	125	1	-	1/5/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	OCY	CB-SG-CD	4.11	114.47	102.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	125	OCY	SG-CD-CE-OZ

There are no ring outliers.

No monomer is involved in short contacts.

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	1.89	2 (13%)	19,20,20	1.80	6 (31%)

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	-	-	2/9/19/19	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	5.51	1.68	1.47
3	A	261	EPE	C10-S	3.47	1.82	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	261	EPE	O3S-S-O1S	-4.40	100.38	111.40
3	A	261	EPE	C3-C2-N1	2.76	116.22	110.65
3	A	261	EPE	C2-C3-N4	2.42	115.54	110.65
3	A	261	EPE	O2S-S-C10	2.38	110.33	106.73
3	A	261	EPE	C7-N4-C3	2.26	117.27	111.24
3	A	261	EPE	C6-N1-C2	2.24	113.67	108.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	261	EPE	C8-C7-N4-C3
3	A	261	EPE	C10-C9-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

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

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.