Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 11:20 PM EDT

PDB ID : 1VSL
Title : ASV INTEGRASE CORE DOMAIN D64N MUTATION WITH ZINC CATION
Authors : Lubkowski, J.; Yang, F.; Alexandratos, J.; Wlodawer, A.
Deposited on : 1998-09-18
Resolution : 2.20 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 (i) 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 (i)) were used in the production of this report:

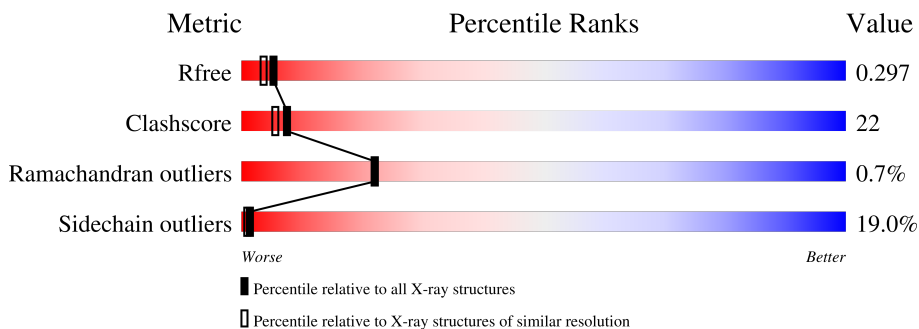|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	Percentile Ranks	Value
Rfree		0.297
Clashscore		22
Ramachandran outliers		0.7%
Sidechain outliers		19.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	146	68% 24% 7% •

WORLDWIDE

wwPDB

PROTEIN DATA BANK

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 1227 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 PROTEIN (INTEGRASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1125	709	211	200	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ASN	ASP	engineered mutation	UNP P03354
A	101	ALA	VAL	SEE REMARK 999	UNP P03354
A	166	LYS	ARG	SEE REMARK 999	UNP P03354

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		

3 Residue-property plots ⓘ

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.

• Molecule 1: PROTEIN (INTEGRASE)

Chain A:
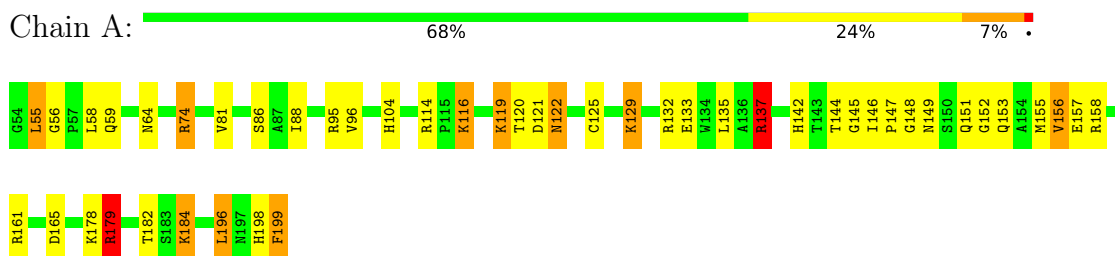
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	67.16Å 67.16Å 79.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 19.89 – 2.19	Depositor EDS
% Data completeness (in resolution range)	86.8 (8.00-2.20) 90.5 (19.89-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.19Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.156 , 0.244 0.250 , 0.297	Depositor DCC
R_{free} test set	914 reflections (10.25%)	wwPDB-VP
Wilson B-factor (Å²)	26.1	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.30 , 94.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	1227	wwPDB-VP
Average B, all atoms (Å²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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

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	0.74	0/1150	0.84	3/1558 (0.2%)

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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	HIS	CG-CD2-NE2	-5.93	97.92	109.20
1	A	179	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	137	ARG	NE-CZ-NH1	5.31	122.95	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	GLY	Peptide

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	1125	0	1141	50	1
2	A	2	0	0	0	0
3	A	100	0	0	4	0
All	All	1227	0	1141	50	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 22.

All (50) 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:119:LYS:HE2	1:A:153:GLN:HG2	1.73	0.70
1:A:119:LYS:HE3	1:A:120:THR:O	1.92	0.70
1:A:121:ASP:HA	1:A:145:GLY:O	1.91	0.70
1:A:198:HIS:O	1:A:199:PHE:OXT	2.11	0.68
1:A:122:ASN:HD22	1:A:122:ASN:N	1.92	0.67
1:A:137:ARG:CG	1:A:137:ARG:HH11	2.08	0.67
1:A:119:LYS:HD2	1:A:152:GLY:O	1.94	0.66
1:A:137:ARG:HH11	1:A:137:ARG:HG3	1.60	0.66
1:A:114:ARG:HD2	3:A:248:HOH:O	1.96	0.65
1:A:119:LYS:HD2	1:A:152:GLY:HA3	1.78	0.64
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.62	0.64
1:A:122:ASN:ND2	1:A:146:ILE:HA	2.14	0.62
1:A:179:ARG:NH2	1:A:182:THR:OG1	2.34	0.61
1:A:129:LYS:HE2	1:A:133:GLU:HB2	1.84	0.60
1:A:119:LYS:HD2	1:A:152:GLY:CA	2.32	0.59
1:A:137:ARG:HH11	1:A:137:ARG:CB	2.17	0.57
1:A:119:LYS:HZ1	1:A:145:GLY:HA3	1.70	0.56
1:A:81:VAL:HG23	1:A:156:VAL:HG23	1.89	0.55
1:A:137:ARG:HH11	1:A:137:ARG:HB2	1.73	0.54
1:A:146:ILE:CD1	1:A:147:PRO:HD2	2.38	0.53
1:A:122:ASN:HD22	1:A:122:ASN:H	1.55	0.52
1:A:120:THR:OG1	1:A:142:HIS:HE1	1.93	0.52
1:A:55:LEU:N	1:A:55:LEU:HD23	2.23	0.51
1:A:146:ILE:HD12	1:A:147:PRO:HD2	1.93	0.51
1:A:125:CYS:SG	3:A:252:HOH:O	2.46	0.51
1:A:74:ARG:HG2	1:A:74:ARG:NH1	2.25	0.50
1:A:146:ILE:HG13	1:A:147:PRO:HD2	1.92	0.50
1:A:122:ASN:N	1:A:122:ASN:ND2	2.58	0.50
1:A:58:LEU:HA	3:A:275:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HD21	1:A:146:ILE:HA	1.78	0.48
1:A:122:ASN:HD21	1:A:145:GLY:C	2.18	0.47
1:A:161:ARG:HB3	1:A:161:ARG:CZ	2.44	0.47
1:A:132:ARG:HG2	3:A:274:HOH:O	2.15	0.47
1:A:119:LYS:C	1:A:119:LYS:HD3	2.35	0.46
1:A:88:ILE:HD13	1:A:196:LEU:HD12	1.97	0.46
1:A:122:ASN:HD21	1:A:146:ILE:N	2.12	0.46
1:A:146:ILE:CG1	1:A:147:PRO:HD2	2.46	0.45
1:A:119:LYS:HE3	1:A:120:THR:C	2.37	0.45
1:A:184:LYS:HE3	1:A:184:LYS:HB3	1.83	0.44
1:A:119:LYS:CD	1:A:152:GLY:O	2.64	0.43
1:A:129:LYS:CE	1:A:133:GLU:HB2	2.47	0.43
1:A:119:LYS:CD	1:A:152:GLY:HA3	2.48	0.43
1:A:122:ASN:ND2	1:A:145:GLY:O	2.52	0.43
1:A:119:LYS:HD2	1:A:152:GLY:C	2.39	0.43
1:A:119:LYS:NZ	1:A:145:GLY:HA3	2.34	0.43
1:A:148:GLY:C	1:A:153:GLN:HB2	2.39	0.43
1:A:59:GLN:HB2	1:A:116:LYS:HG2	2.00	0.42
1:A:137:ARG:HG3	1:A:137:ARG:NH1	2.31	0.42
1:A:122:ASN:HD21	1:A:146:ILE:CA	2.33	0.42
1:A:135:LEU:HD13	1:A:142:HIS:HB2	2.02	0.42

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:95:ARG:NH2	1:A:199:PHE:OXT[4_565]	2.01	0.19

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	144/146 (99%)	134 (93%)	9 (6%)	1 (1%)	22	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ASN

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	116/116 (100%)	94 (81%)	22 (19%)	1	1

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	64	ASN
1	A	74	ARG
1	A	86	SER
1	A	96	VAL
1	A	116	LYS
1	A	119	LYS
1	A	122	ASN
1	A	129	LYS
1	A	137	ARG
1	A	144	THR
1	A	151	GLN
1	A	155	MET
1	A	156	VAL
1	A	157	GLU
1	A	158	ARG
1	A	165	ASP
1	A	178	LYS
1	A	179	ARG
1	A	184	LYS

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Mol	Chain	Res	Type
1	A	196	LEU
1	A	199	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	122	ASN
1	A	142	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.