



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2023 – 06:47 PM JST

PDB ID : 5GVU
Title : crystal structure of BVDV NS3 helicase domain
Authors : Li, S.; Mao, X.
Deposited on : 2016-09-06
Resolution : 2.82 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

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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

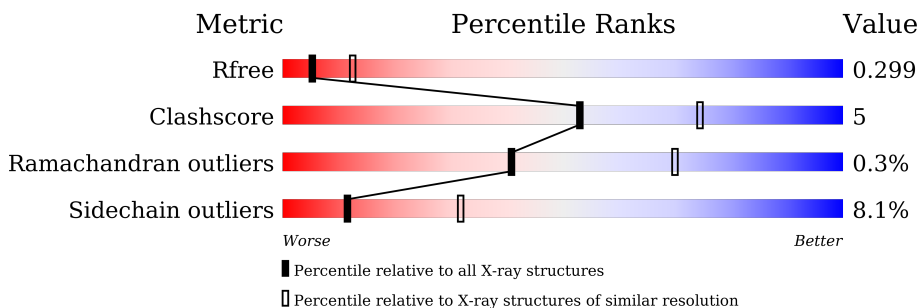
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	476	78% (green), 16% (yellow), 5% (orange), 1% (red), 0% (grey)
1	B	476	60% (green), 13% (yellow), 25% (orange), 2% (red), 0% (grey)
1	C	476	66% (green), 12% (yellow), 21% (orange), 1% (red), 0% (grey)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9452 atoms, of which 0 are hydrogens and 0 are deuteriums.

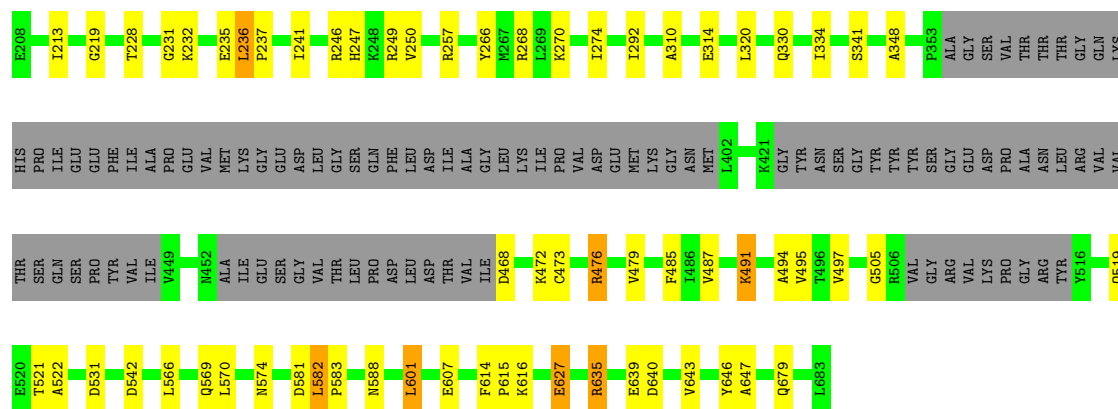
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NS3 helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	Total 3596	C 2289	N 609	O 680	S 18	0	0	0
1	B	355	Total 2824	C 1792	N 481	O 537	S 14	0	0	0
1	C	377	Total 2994	C 1902	N 512	O 565	S 15	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total 15	O 15	0	0
2	B	13	Total 13	O 13	0	0
2	C	10	Total 10	O 10	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	121.10Å 121.10Å 109.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 2.82 48.61 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.01-2.82) 99.9 (48.61-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.90 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0124, REFMAC 5.8.0124	Depositor
R, R_{free}	0.272 , 0.298 0.272 , 0.299	Depositor DCC
R_{free} test set	2121 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	0.119 for -h,-k,l 0.119 for h,-h-k,-l 0.390 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9452	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/3661	0.66	0/4949
1	B	0.41	0/2875	0.69	0/3886
1	C	0.43	0/3046	0.68	1/4115 (0.0%)
All	All	0.42	0/9582	0.68	1/12950 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	601	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3596	0	3626	39	0
1	B	2824	0	2833	36	0
1	C	2994	0	3025	28	0
2	A	15	0	0	0	0
2	B	13	0	0	0	0
2	C	10	0	0	0	0
All	All	9452	0	9484	102	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 5.

The worst 5 of 102 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:635:ARG:NH2	1:B:640:ASP:O	2.15	0.79
1:A:463:LEU:HG	1:A:507:VAL:HG12	1.64	0.78
1:C:476:ARG:HH11	1:C:476:ARG:HG3	1.53	0.72
1:A:392:ILE:HD11	1:A:467:ILE:HD13	1.72	0.72
1:A:463:LEU:HG	1:A:507:VAL:CG1	2.20	0.70

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	442/476 (93%)	426 (96%)	14 (3%)	2 (0%)	29	59
1	B	347/476 (73%)	333 (96%)	14 (4%)	0	100	100
1	C	367/476 (77%)	353 (96%)	13 (4%)	1 (0%)	41	70
All	All	1156/1428 (81%)	1112 (96%)	41 (4%)	3 (0%)	41	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	505	GLY
1	A	231	GLY
1	A	406	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	391/407 (96%)	356 (91%)	35 (9%)	9	27
1	B	307/407 (75%)	284 (92%)	23 (8%)	13	35
1	C	325/407 (80%)	300 (92%)	25 (8%)	13	34
All	All	1023/1221 (84%)	940 (92%)	83 (8%)	11	32

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	683	LEU
1	C	542	ASP
1	C	247	HIS
1	C	476	ARG
1	C	582	LEU

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	C	265	GLN
1	C	324	HIS
1	C	669	GLN
1	C	569	GLN
1	A	633	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 monosaccharides 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

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.