

# Full wwPDB X-ray Structure Validation Report (i)

### Oct 3, 2023 – 12:47 AM EDT

PDB ID : 6OXW

Title: HIV-1 Protease NL4-3 WT in Complex with LR-100

Authors: Lockbaum, G.J.; Rusere, L.N.; Lee, S.K.; Henes, M.; Kosovrasti, K.; Spielvo-

gel, E.; Nalivaika, E.A.; Swanstrom, R.; KurtYilmaz, N.; Schiffer, C.A.; Ali,

Α.

Deposited on : 2019-05-14

Resolution : 1.98 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 (1)) were used in the production of this report:

MolProbity : FAILED

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.98 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3222 atoms, of which 1542 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.

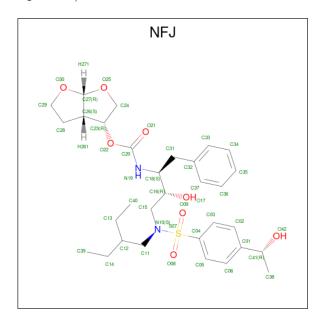
• Molecule 1 is a protein called Protease NL4-3.

Mol	Chain	Residues			Aton	ns			ZeroOcc	AltConf	Trace
1	В	99	Total 1490	C 473	H 756	N 126	O 131	S 4	0	1	0
1	A	99	Total 1479	C 478	H 742	N 124	O 131	S 4	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	7	LYS	GLN	engineered mutation	UNP Q8ULI9
A	7	LYS	GLN	engineered mutation	UNP Q8ULI9

• Molecule 2 is (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl {(2S,3R)-4-[(2-ethylbutyl)( {4-[(1R)-1-hydroxyethyl]phenyl}sulfonyl)amino]-3-hydroxy-1-phenylbutan-2-yl}carba mate (three-letter code: NFJ) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>2</sub>O<sub>8</sub>S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		A	tom	ıs			ZeroOcc	AltConf
9	Λ	1	Total	С	Н	N	О	S	0	0
	Λ	1	86	31	44	2	8	1	0	

### • Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	85	Total O 85 85	0	0
3	A	82	Total O 82 82	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	50.92Å 58.88Å 61.68Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	27.32 - 1.98	Depositor
% Data completeness	95.3 (27.32-1.98)	Depositor
(in resolution range)	,	-
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.32 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
$R, R_{free}$	0.188 , $0.238$	Depositor
Wilson B-factor $(A^2)$	24.3	Xtriage
Anisotropy	0.277	Xtriage
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.037 for -h,l,k	Xtriage
Total number of atoms	3222	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 4 Model quality (i)

# 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

# 4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

# 4.6 Ligand geometry (i)

1 ligand 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).

Mo	Type	Chain	Res	Link	В	ond leng	$\operatorname{gths}$	В	ond ang	gles
IVIO	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NFJ	A	101	-	45,45,45	5.34	28 (62%)	56,63,63	2.18	11 (19%)

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.

$\mathbf{Mol}$	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NFJ	A	101	-	-	2/44/63/63	0/4/4/4

All (28) bond length outliers are listed below:

2       A       101       NFJ       C05-C04       11.15       1.56         2       A       101       NFJ       C26-C23       -10.27       1.34         2       A       101       NFJ       C06-C01       9.98       1.55         2       A       101       NFJ       C02-C01       9.62       1.54         2       A       101       NFJ       S07-N10       9.02       1.76         2       A       101       NFJ       C03-C04       8.96       1.52         2       A       101       NFJ       C03-C02       8.30       1.53         2       A       101       NFJ       C04-S07       7.82       1.87         2       A       101       NFJ       C34-C33       7.60       1.54         2       A       101       NFJ       C36-C37       7.45       1.54         2       A       101       NFJ       C26-C35       7.13       1.51         2       A       101       NFJ       C37-C32       7.08       1.54         2       A       101       NFJ       C33-C32       7.01       1.54         2	1.38 1.53 1.39 1.39 1.63
2       A       101       NFJ       C06-C01       9.98       1.55         2       A       101       NFJ       C02-C01       9.62       1.54         2       A       101       NFJ       S07-N10       9.02       1.76         2       A       101       NFJ       C03-C04       8.96       1.52         2       A       101       NFJ       C03-C02       8.30       1.53         2       A       101       NFJ       C04-S07       7.82       1.87         2       A       101       NFJ       C34-C33       7.60       1.54         2       A       101       NFJ       C36-C37       7.45       1.54         2       A       101       NFJ       C06-C05       7.13       1.51         2       A       101       NFJ       C28-C26       -7.10       1.35         2       A       101       NFJ       C37-C32       7.08       1.54         2       A       101       NFJ       C33-C32       7.01       1.54         2       A       101       NFJ       C20-N19       6.09       1.49	1.39 1.39
2       A       101       NFJ       C02-C01       9.62       1.54         2       A       101       NFJ       S07-N10       9.02       1.76         2       A       101       NFJ       C03-C04       8.96       1.52         2       A       101       NFJ       C03-C02       8.30       1.53         2       A       101       NFJ       C04-S07       7.82       1.87         2       A       101       NFJ       C34-C33       7.60       1.54         2       A       101       NFJ       C36-C37       7.45       1.54         2       A       101       NFJ       C06-C05       7.13       1.51         2       A       101       NFJ       C28-C26       -7.10       1.35         2       A       101       NFJ       C37-C32       7.08       1.54         2       A       101       NFJ       C33-C32       7.01       1.54         2       A       101       NFJ       C20-N19       6.09       1.49	1.39
2       A       101       NFJ       S07-N10       9.02       1.76         2       A       101       NFJ       C03-C04       8.96       1.52         2       A       101       NFJ       C03-C02       8.30       1.53         2       A       101       NFJ       C04-S07       7.82       1.87         2       A       101       NFJ       C34-C33       7.60       1.54         2       A       101       NFJ       C36-C37       7.45       1.54         2       A       101       NFJ       C06-C05       7.13       1.51         2       A       101       NFJ       C28-C26       -7.10       1.35         2       A       101       NFJ       C37-C32       7.08       1.54         2       A       101       NFJ       C33-C32       7.01       1.54         2       A       101       NFJ       C20-N19       6.09       1.49	
2       A       101       NFJ       C03-C04       8.96       1.52         2       A       101       NFJ       C03-C02       8.30       1.53         2       A       101       NFJ       C04-S07       7.82       1.87         2       A       101       NFJ       C34-C33       7.60       1.54         2       A       101       NFJ       C36-C37       7.45       1.54         2       A       101       NFJ       C06-C05       7.13       1.51         2       A       101       NFJ       C28-C26       -7.10       1.35         2       A       101       NFJ       C37-C32       7.08       1.54         2       A       101       NFJ       C33-C32       7.01       1.54         2       A       101       NFJ       C20-N19       6.09       1.49	1.63
2       A       101       NFJ       C03-C02       8.30       1.53         2       A       101       NFJ       C04-S07       7.82       1.87         2       A       101       NFJ       C34-C33       7.60       1.54         2       A       101       NFJ       C36-C37       7.45       1.54         2       A       101       NFJ       C06-C05       7.13       1.51         2       A       101       NFJ       C28-C26       -7.10       1.35         2       A       101       NFJ       C37-C32       7.08       1.54         2       A       101       NFJ       C33-C32       7.01       1.54         2       A       101       NFJ       C20-N19       6.09       1.49	1.00
2     A     101     NFJ     C04-S07     7.82     1.87       2     A     101     NFJ     C34-C33     7.60     1.54       2     A     101     NFJ     C36-C37     7.45     1.54       2     A     101     NFJ     C06-C05     7.13     1.51       2     A     101     NFJ     C28-C26     -7.10     1.35       2     A     101     NFJ     C37-C32     7.08     1.54       2     A     101     NFJ     C33-C32     7.01     1.54       2     A     101     NFJ     C20-N19     6.09     1.49	1.38
2     A     101     NFJ     C34-C33     7.60     1.54       2     A     101     NFJ     C36-C37     7.45     1.54       2     A     101     NFJ     C06-C05     7.13     1.51       2     A     101     NFJ     C28-C26     -7.10     1.35       2     A     101     NFJ     C37-C32     7.08     1.54       2     A     101     NFJ     C33-C32     7.01     1.54       2     A     101     NFJ     C20-N19     6.09     1.49	1.38
2     A     101     NFJ     C36-C37     7.45     1.54       2     A     101     NFJ     C06-C05     7.13     1.51       2     A     101     NFJ     C28-C26     -7.10     1.35       2     A     101     NFJ     C37-C32     7.08     1.54       2     A     101     NFJ     C33-C32     7.01     1.54       2     A     101     NFJ     C20-N19     6.09     1.49	1.76
2     A     101     NFJ     C06-C05     7.13     1.51       2     A     101     NFJ     C28-C26     -7.10     1.35       2     A     101     NFJ     C37-C32     7.08     1.54       2     A     101     NFJ     C33-C32     7.01     1.54       2     A     101     NFJ     C20-N19     6.09     1.49	1.38
2     A     101     NFJ     C28-C26     -7.10     1.35       2     A     101     NFJ     C37-C32     7.08     1.54       2     A     101     NFJ     C33-C32     7.01     1.54       2     A     101     NFJ     C20-N19     6.09     1.49	1.38
2     A     101     NFJ     C37-C32     7.08     1.54       2     A     101     NFJ     C33-C32     7.01     1.54       2     A     101     NFJ     C20-N19     6.09     1.49	1.38
2     A     101     NFJ     C33-C32     7.01     1.54       2     A     101     NFJ     C20-N19     6.09     1.49	1.54
2 A 101 NFJ C20-N19 6.09 1.49	1.38
	1.38
2 A 101 NET C36 C35 6 07 1 54	1.34
2   A   101   NF3   C50-C55   0.07   1.54	1.38
2 A 101 NFJ C35-C34 6.04 1.54	1.38
2 A 101 NFJ 008-S07 5.57 1.49	1.43
2 A 101 NFJ O25-C27 4.11 1.50	1.41
2 A 101 NFJ O30-C27 3.95 1.50	1.41
2 A 101 NFJ O22-C20 3.77 1.41	1.35
2 A 101 NFJ 009-S07 3.57 1.47	1.43
2 A 101 NFJ C31-C32 3.43 1.59	1.51
2 A 101 NFJ C27-C26 2.70 1.57	1.52
2 A 101 NFJ O25-C24 -2.60 1.38	1.43

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$Ideal(\AA)$
2	A	101	NFJ	O22-C23	2.50	1.50	1.46
2	A	101	NFJ	C24-C23	2.39	1.57	1.52
2	A	101	NFJ	C28-C29	2.03	1.56	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
2	A	101	NFJ	O09-S07-O08	-9.64	103.90	119.52
2	A	101	NFJ	O09-S07-N10	6.27	112.40	106.69
2	A	101	NFJ	O08-S07-N10	5.91	112.08	106.69
2	A	101	NFJ	O22-C20-N19	4.08	115.61	110.32
2	A	101	NFJ	O09-S07-C04	3.45	112.41	108.05
2	A	101	NFJ	C32-C31-C18	-2.79	108.49	113.33
2	A	101	NFJ	O08-S07-C04	2.70	111.46	108.05
2	A	101	NFJ	C29-C28-C26	2.63	107.01	103.32
2	A	101	NFJ	C31-C18-N19	-2.33	106.68	110.07
2	A	101	NFJ	C04-S07-N10	-2.10	104.80	107.30
2	A	101	NFJ	C06-C01-C02	2.04	120.83	118.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

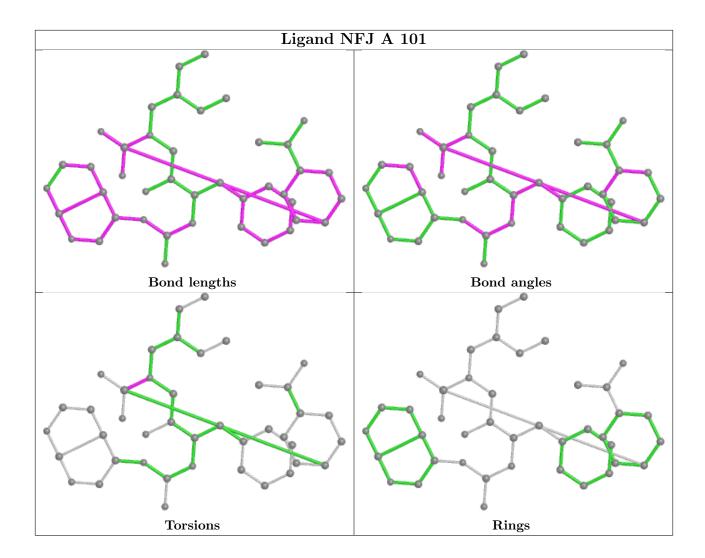
Mol	Chain	Res	Type	Atoms
2	A	101	NFJ	C11-N10-S07-O08
2	A	101	NFJ	C15-N10-S07-O08

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





# 4.7 Other polymers (i)

There are no such residues in this entry.

# 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

### 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

# 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

