



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 08:28 AM EDT

PDB ID : 2FGV  
Title : X-ray crystal structure of HIV-1 Protease T80N variant in complex with the inhibitor saquinavir used to explore the role of invariant Thr80 in HIV-1 protease structure, function, and viral infectivity.  
Authors : Foulkes, J.E.; Prabu-Jeyabalan, M.; Cooper, D.; Schiffer, C.A.  
Deposited on : 2005-12-22  
Resolution : 1.50 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.23.2

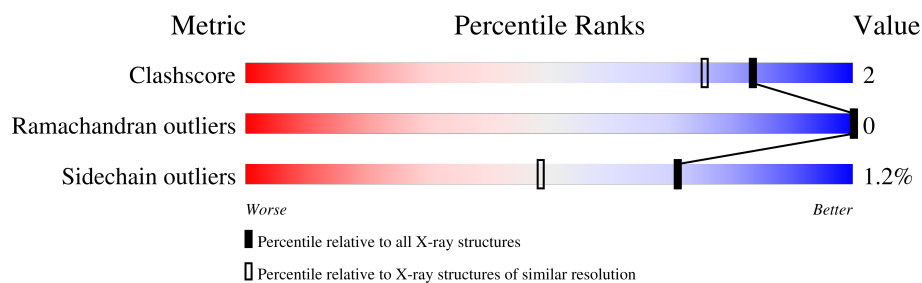
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

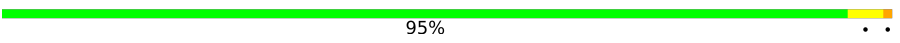

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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  $\geq 3$ , 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	99	 95% . .
1	B	99	 92% 8%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 1847 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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	3	0
			778	500	136	137	5			
1	B	99	Total	C	N	O	S	0	5	0
			787	505	137	141	4			

There are 6 discrepancies between the modelled and reference sequences:

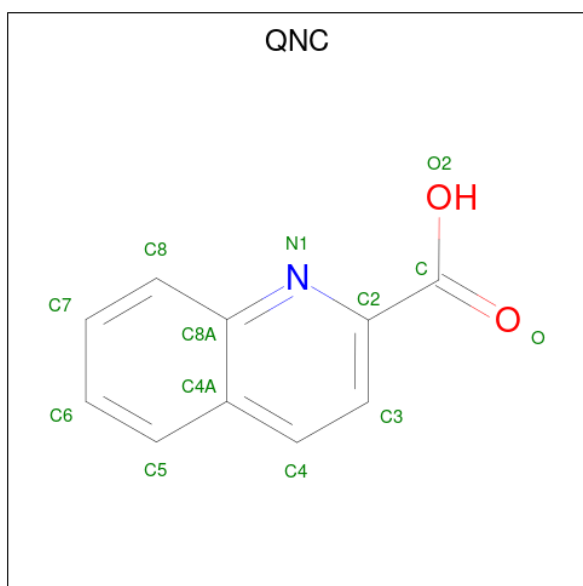
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	GLN	engineered mutation	UNP O38716
A	64	VAL	ILE	engineered mutation	UNP O38716
A	80	ASN	THR	engineered mutation	UNP O38716
B	7	LYS	GLN	engineered mutation	UNP O38716
B	64	VAL	ILE	engineered mutation	UNP O38716
B	80	ASN	THR	engineered mutation	UNP O38716

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



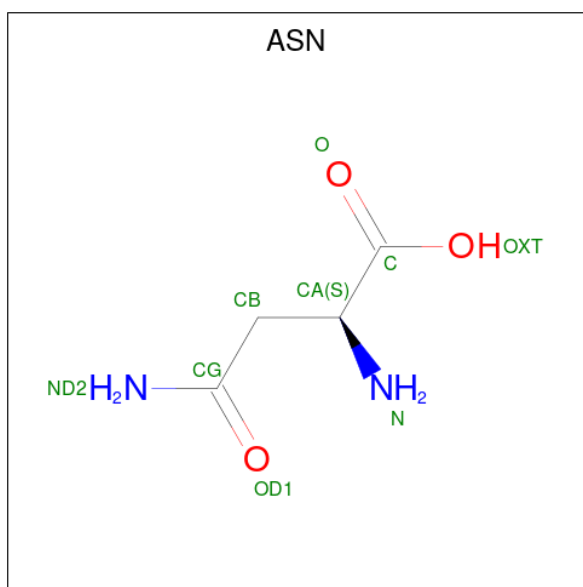
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	1
			10	8	2		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is quinoline-2-carboxylic acid (three-letter code: QNC) (formula:  $C_{10}H_7NO_2$ ).



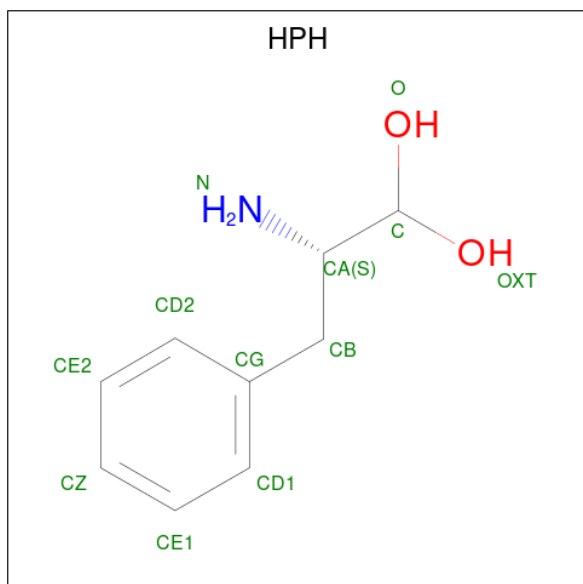
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	10	1	1		

- Molecule 4 is ASPARAGINE (three-letter code: ASN) (formula:  $C_4H_8N_2O_3$ ).



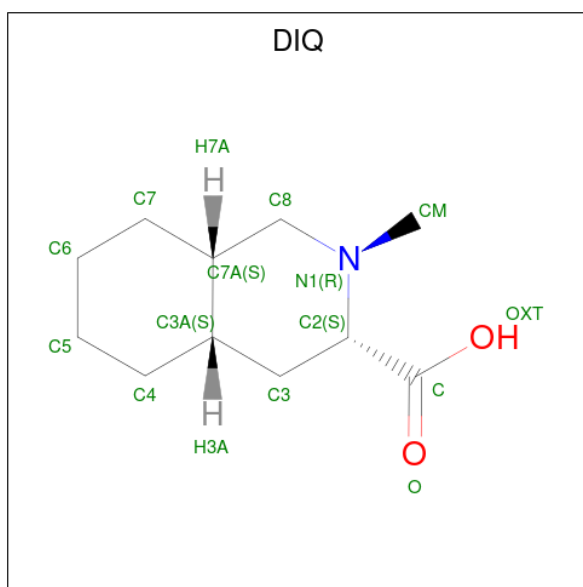
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 5 is (2S)-2-amino-3-phenylpropane-1,1-diol (three-letter code: HPH) (formula:  $C_9H_{13}NO_2$ ).



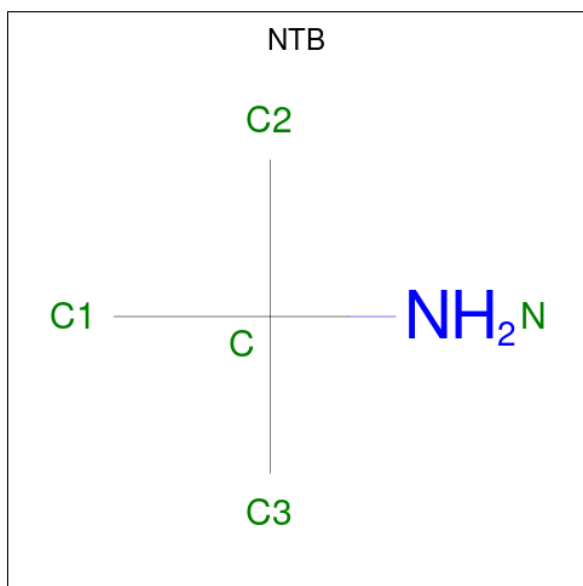
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 6 is 2-METHYL-DECAHYDRO-ISOQUINOLINE-3-CARBOXYLIC ACID (three-letter code: DIQ) (formula:  $C_{11}H_{19}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			13	11	1	1		

- Molecule 7 is TERTIARY-BUTYLAMINE (three-letter code: NTB) (formula:  $C_4H_{11}N$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	97	Total 97	O 97	0	0
8	B	96	Total 96	O 96	0	0

### 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: Protease

Chain A:  95% ..



- Molecule 1: Protease

Chain B:  92% 8%





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.52Å 58.18Å 61.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.26 – 1.50	Depositor
% Data completeness (in resolution range)	99.4 (42.26-1.50)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.171 , 0.197	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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: DIQ, NTB, QNC, HPH, PO4

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	0.28	0/792	0.60	0/1074
1	B	0.26	0/801	0.64	0/1088
All	All	0.27	0/1593	0.62	0/2162

There are no bond length outliers.

There are no bond angle outliers.

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	778	0	814	4	0
1	B	787	0	808	4	0
2	A	25	0	0	0	0
2	B	15	0	0	0	0
3	A	12	0	6	0	0
4	A	8	0	5	0	0
5	A	11	0	8	0	0
6	A	13	0	16	0	0
7	A	5	0	10	1	0
8	A	97	0	0	0	0
8	B	96	0	0	2	0
All	All	1847	0	1667	8	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 2.

All (8) 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:80:ASN:CG	8:B:602:HOH:O	2.35	0.63
1:A:50[A]:ILE:HG12	7:A:512:NTB:H22	1.81	0.62
1:B:14[B]:ARG:HH12	1:B:65[B]:GLU:CD	2.09	0.55
1:B:20:LYS:HE3	1:B:36:MET:SD	2.51	0.50
1:A:46[A]:MET:SD	1:A:55:LYS:HG2	2.57	0.45
1:B:23:LEU:HD23	1:B:84[B]:ILE:CD1	2.48	0.43
1:A:11:VAL:HB	1:A:67:CYS:SG	2.58	0.43
1:A:50[B]:ILE:HD13	8:B:602:HOH:O	2.20	0.42

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	100/99 (101%)	98 (98%)	2 (2%)	0	100	100
1	B	102/99 (103%)	102 (100%)	0	0	100	100
All	All	202/198 (102%)	200 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	84/83 (101%)	82 (98%)	2 (2%)	49	19
1	B	84/83 (101%)	83 (99%)	1 (1%)	71	48
All	All	168/166 (101%)	165 (98%)	3 (2%)	71	30

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50[A]	ILE
1	A	50[B]	ILE
1	B	61	GLN

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	18	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 ligands are 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	$\# Z  > 2$
2	PO4	A	503	-	4,4,4	0.92	0	6,6,6	0.50	0
3	QNC	A	508	4	13,13,14	1.28	1 (7%)	17,17,19	2.33	5 (29%)
2	PO4	A	502	-	4,4,4	1.03	0	6,6,6	0.76	0
6	DIQ	A	511	5,7	12,14,15	0.67	1 (8%)	15,19,21	1.41	3 (20%)
2	PO4	B	504	-	4,4,4	0.88	0	6,6,6	0.42	0
7	NTB	A	512	6	4,4,4	0.59	0	6,6,6	0.32	0
4	ASN	A	509	3,5	6,7,8	0.74	0	5,8,10	2.02	2 (40%)
2	PO4	A	507[A]	-	4,4,4	0.92	0	6,6,6	0.29	0
2	PO4	A	501	-	4,4,4	0.87	0	6,6,6	0.54	0
5	HPH	A	510	4,6	11,11,12	0.74	0	11,13,15	1.04	1 (9%)
2	PO4	A	507[B]	-	4,4,4	0.90	0	6,6,6	0.39	0
2	PO4	B	505	-	4,4,4	0.89	0	6,6,6	0.40	0
2	PO4	B	506	-	4,4,4	0.93	0	6,6,6	0.48	0

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	QNC	A	508	4	-	0/2/2/4	0/2/2/2
5	HPH	A	510	4,6	-	0/6/6/8	0/1/1/1
6	DIQ	A	511	5,7	-	1/1/25/27	0/2/2/2
4	ASN	A	509	3,5	-	1/5/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	QNC	C2-N1	2.41	1.35	1.33
6	A	511	DIQ	CM-N1	-2.12	1.42	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	QNC	C-C2-N1	6.59	121.11	114.66
4	A	509	ASN	CA-CB-CG	-3.66	104.97	112.24
3	A	508	QNC	C3-C2-C	-3.31	118.24	121.19
3	A	508	QNC	C2-N1-C8A	3.20	120.73	117.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	QNC	O-C-C2	-2.98	121.40	124.22
6	A	511	DIQ	C8-C7A-C3A	2.88	113.88	108.17
6	A	511	DIQ	C8-N1-C2	-2.86	107.69	110.88
4	A	509	ASN	CB-CA-C	2.59	116.33	111.47
5	A	510	HPH	CB-CA-C	-2.57	107.56	112.21
6	A	511	DIQ	C7-C7A-C8	-2.54	108.89	111.93
3	A	508	QNC	C5-C4A-C8A	2.21	121.57	118.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	509	ASN	O-C-CA-CB
6	A	511	DIQ	O-C-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	512	NTB	1	0

## 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.