

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

#### Oct 4, 2023 – 10:58 PM EDT

PDB ID : 6UTD

Title : CRYSTAL STRUCTURE OF UNLIGANDED HIV-1 LM/HS CLADE A/E

CRF01 GP120 CORE

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Deposited on : 2019-10-29

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 : FAILED

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

Xtriage (Phenix) : 1.13 EDS : FAILED

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-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 4 unique types of molecules in this entry. The entry contains 2856 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 HIV-1 LM/HS clade A/E CRF01 gp120 core.

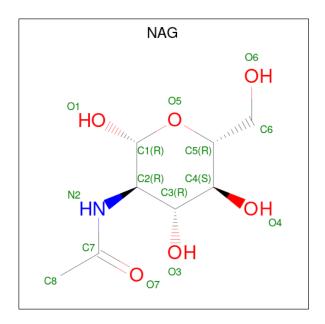
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	340	Total 2668	C 1675	N 461	O 509	S 23	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
A	42	VAL	-	expression tag	UNP A0A0M3KKW9	
A	43	PRO	=	expression tag	UNP A0A0M3KKW9	
A	61	TYR	HIS	engineered mutation	UNP A0A0M3KKW9	
A	105	HIS	GLN	engineered mutation	UNP A0A0M3KKW9	
A	108	ILE	VAL	engineered mutation	UNP A0A0M3KKW9	
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9	
A	474	ASP	ASN	engineered mutation	UNP A0A0M3KKW9	
A	475	MET	ILE	engineered mutation	UNP A0A0M3KKW9	
A	476	ARG	LYS	engineered mutation	UNP A0A0M3KKW9	

• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

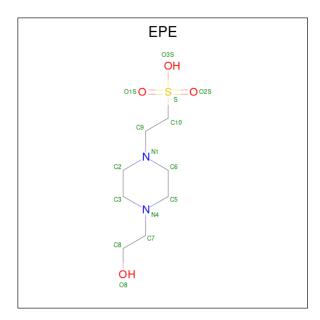




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0

 $\bullet$  Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANE SULFONIC ACID (three-letter code: EPE) (formula:  $\rm C_8H_{18}N_2O_4S).$ 





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
9	Λ	1	Total	С	N	О	S	0	0
3	A	1	15	8	2	4	1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	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	63.96Å 65.63Å 87.78Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	45.80 - 2.20	Depositor	
% Data completeness	88.5 (45.80-2.20)	Depositor	
(in resolution range)	` ,	-	
$R_{merge}$	0.11	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.03  (at  2.18Å)	Xtriage	
Refinement program	PHENIX (1.15.2_3472: ???), REFMAC 5.8.0257	Depositor	
$R, R_{free}$	0.228 , $0.270$	Depositor	
Wilson B-factor $(A^2)$	52.2	Xtriage	
Anisotropy	0.475	Xtriage	
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	0.009 for k,h,-l	Xtriage	
Total number of atoms	2856	wwPDB-VP	
Average B, all atoms $(\mathring{A}^2)$	64.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.17% 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)

11 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).

Mal	Trino	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
Mol	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	507	1	14,14,15	1.19	1 (7%)	17,19,21	1.23	2 (11%)
2	NAG	A	505	1	14,14,15	0.32	0	17,19,21	0.55	0
3	EPE	A	511	-	15,15,15	0.75	1 (6%)	18,20,20	1.82	5 (27%)
2	NAG	A	501	1	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	A	508	1	14,14,15	0.46	0	17,19,21	0.42	0
2	NAG	A	504	1	14,14,15	0.47	0	17,19,21	0.47	0
2	NAG	A	502	1	14,14,15	0.64	0	17,19,21	0.46	0
2	NAG	A	509	1	14,14,15	0.46	0	17,19,21	1.62	1 (5%)
2	NAG	A	506	1	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	A	510	1	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
2	NAG	A	503	1	14,14,15	0.41	0	17,19,21	0.54	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
2	NAG	A	507	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
3	EPE	A	511	_	-	7/9/19/19	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	502	1	-	1/6/23/26	0/1/1/1
2	NAG	A	509	1	-	1/6/23/26	0/1/1/1
2	NAG	A	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	510	1	-	1/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

	Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
	2	A	507	NAG	O5-C1	-4.29	1.36	1.43
ĺ	3	A	511	EPE	C10-S	2.45	1.81	1.77

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
2	A	509	NAG	C1-O5-C5	5.90	120.18	112.19
3	A	511	EPE	C5-N4-C3	3.46	116.62	108.83
2	A	510	NAG	C1-O5-C5	3.28	116.64	112.19
3	A	511	EPE	C7-N4-C5	3.14	119.27	111.23
2	A	507	NAG	C4-C3-C2	3.11	115.57	111.02
3	A	511	EPE	C7-N4-C3	2.94	118.75	111.23
2	A	507	NAG	C3-C4-C5	2.76	115.16	110.24
3	A	511	EPE	C9-N1-C6	-2.53	104.76	111.23
3	A	511	EPE	O1S-S-C10	2.36	109.75	106.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	511	EPE	C8-C7-N4-C5
3	A	511	EPE	C9-C10-S-O2S
3	A	511	EPE	C9-C10-S-O3S
2	A	506	NAG	O5-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	A	509	NAG	O5-C5-C6-O6
3	A	511	EPE	S-C10-C9-N1
2	A	510	NAG	O5-C5-C6-O6
3	A	511	EPE	C8-C7-N4-C3
3	A	511	EPE	C9-C10-S-O1S
2	A	504	NAG	O5-C5-C6-O6
3	A	511	EPE	N4-C7-C8-O8
2	A	504	NAG	C4-C5-C6-O6
2	A	502	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

### 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.

