Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 12:24 AM EDT

PDB ID	:	6VDM
Title	:	HCV NS3/4A protease A156T, D168E double mutant in complex with glecaprevir
Authors	:	Timm, J.; Schiffer, C.A.
Deposited on	:	2019-12-27
Resolution	:	1.90 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 ⓘ 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	:	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-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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 6 unique types of molecules in this entry. The entry contains 3162 atoms, of which 1391 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 Non-structural protein 4A, Serine protease NS3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	202	2892	925	1391	274	293	9	0	4	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	980	GLY	-	expression tag	UNP P26664
A	981	SER	-	expression tag	UNP P26664
A	982	HIS	-	expression tag	UNP P26664
A	983	MET	-	expression tag	UNP P26664
A	984	ALA	-	expression tag	UNP P26664
A	985	SER	-	expression tag	UNP P26664
A	986	MET	-	expression tag	UNP P26664
A	987	LYS	-	expression tag	UNP P26664
A	988	LYS	-	expression tag	UNP P26664
A	989	LYS	-	expression tag	UNP P26664
A	991	SER	CYS	engineered mutation	UNP P26664
A	998	ILE	VAL	engineered mutation	UNP P26664
A	999	ASN	VAL	engineered mutation	UNP P26664
A	1001	SER	-	linker	UNP P26664
A	1002	GLY	-	linker	UNP P26664
A	1003	ASP	-	linker	UNP P26664
A	1013	GLU	LEU	engineered mutation	UNP P26664
A	1014	GLU	LEU	engineered mutation	UNP P26664
A	1017	GLN	ILE	engineered mutation	UNP P26664
A	1018	GLU	ILE	engineered mutation	UNP P26664
A	1021	GLN	LEU	engineered mutation	UNP P26664
A	1040	THR	ALA	engineered mutation	UNP P26664
A	1047	SER	CYS	engineered mutation	UNP P26664
A	1052	LEU	CYS	engineered mutation	UNP P26664
A	1072	THR	ILE	engineered mutation	UNP P26664
A	1080	LYS	GLN	engineered mutation	UNP P26664
A	1086	GLN	PRO	engineered mutation	UNP P26664

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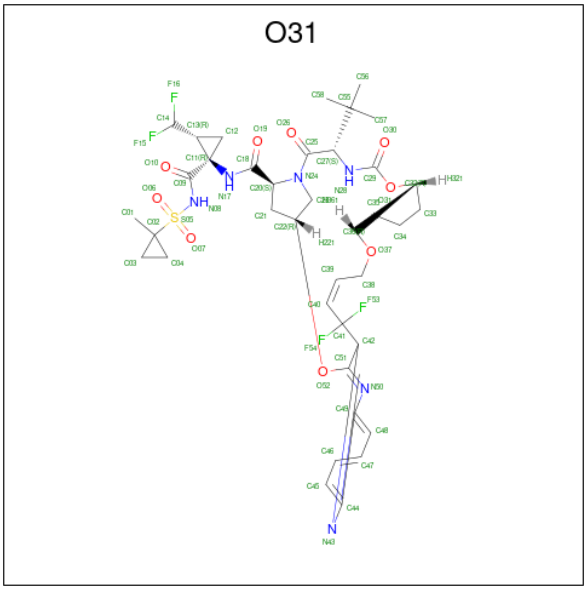
Chain	Residue	Modelled	Actual	Comment	Reference
A	1156	THR	ALA	engineered mutation	UNP P26664
A	1168	GLU	ASP	engineered mutation	UNP P26664
A	1174	SER	ASN	engineered mutation	UNP P26664

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

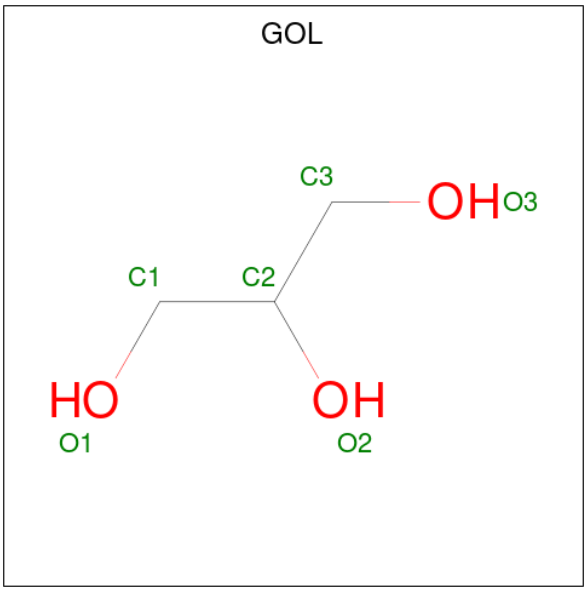
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is (3aR,7S,10S,12R,21E,24aR)-7-tert-butyl-N-[(1R,2R)-2-(difluoromethyl)-1-{[(1-methylcyclopropyl)sulfonyl]carbamoyl}cyclop ropyl]-20,20-difluoro-5,8-dioxo-2,3,3a,5,6,7,8,11,12,20,23,24a-dodecahydro-1H,10H-9,12-methanocyclopenta[18,19][1,10,17, 3,6]trioxadi azacyclononadecino[11,12-b]quinoxaline-10-carboxamide (three-letter code: O31) (formula: $C_{38}H_{46}F_4N_6O_9S$) (labeled as "Ligand of Interest" by depositor).



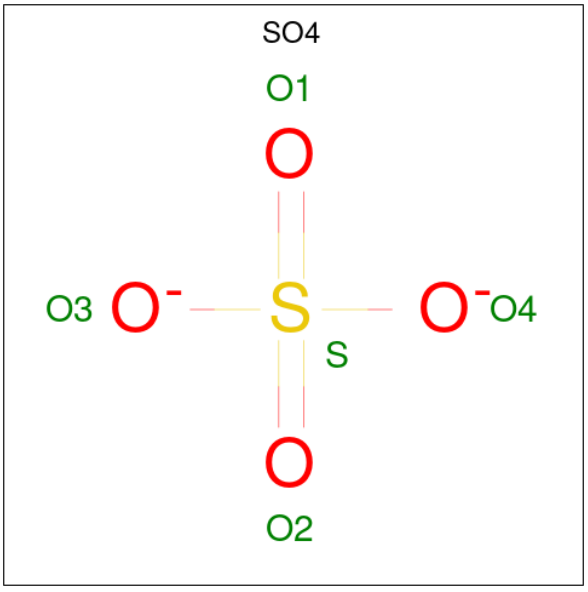
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 58	C 38	F 4	N 6	O 9	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total	O	0	0
			190	190		

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 a, b, c, α, β, γ	54.34Å 58.64Å 60.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.71 – 1.90	Depositor
% Data completeness (in resolution range)	99.4 (23.71-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	20.67 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.162 , 0.196	Depositor
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.426	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
Total number of atoms	3162	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GOL	A	1203	-	5,5,5	1.07	1 (20%)	5,5,5	1.01	0
5	SO4	A	1204	-	4,4,4	0.18	0	6,6,6	0.23	0
3	O31	A	1202	-	58,64,64	3.05	20 (34%)	80,101,101	2.21	19 (23%)
5	SO4	A	1205	-	4,4,4	0.16	0	6,6,6	0.16	0
5	SO4	A	1206	-	4,4,4	0.14	0	6,6,6	0.05	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	O31	A	1202	-	-	3/59/107/107	0/6/7/7
4	GOL	A	1203	-	-	0/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	O31	C42-N43	10.91	1.45	1.30
3	A	1202	O31	C49-N50	9.17	1.52	1.37
3	A	1202	O31	C44-N43	8.86	1.52	1.37
3	A	1202	O31	C18-N17	5.52	1.45	1.34
3	A	1202	O31	C51-N50	5.17	1.43	1.30
3	A	1202	O31	C29-N28	4.92	1.46	1.34
3	A	1202	O31	C25-N24	4.85	1.45	1.34
3	A	1202	O31	O31-C29	4.12	1.42	1.35
3	A	1202	O31	S05-N08	3.59	1.65	1.60
3	A	1202	O31	O31-C32	-3.41	1.40	1.46
3	A	1202	O31	O52-C51	3.07	1.43	1.36
3	A	1202	O31	C02-S05	-2.93	1.79	1.81
3	A	1202	O31	O37-C36	-2.78	1.38	1.43
3	A	1202	O31	C47-C48	2.55	1.42	1.36
3	A	1202	O31	C12-C11	2.51	1.53	1.51
3	A	1202	O31	C23-C22	-2.38	1.48	1.52
3	A	1202	O31	O06-S05	2.30	1.47	1.43
3	A	1202	O31	C23-N24	2.12	1.50	1.47
4	A	1203	GOL	O2-C2	-2.09	1.37	1.43
3	A	1202	O31	O07-S05	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	O31	C04-C03	2.04	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1202	O31	O06-S05-C02	8.32	114.28	107.60
3	A	1202	O31	C09-N08-S05	-8.13	110.95	124.08
3	A	1202	O31	C09-C11-N17	5.86	122.36	116.06
3	A	1202	O31	O07-S05-O06	-4.93	110.57	120.57
3	A	1202	O31	O31-C29-N28	4.52	116.18	110.32
3	A	1202	O31	C51-O52-C22	-3.94	112.90	118.56
3	A	1202	O31	O07-S05-C02	-3.57	104.73	107.60
3	A	1202	O31	C18-C20-N24	-3.46	103.03	112.56
3	A	1202	O31	O10-C09-C11	3.34	124.72	120.74
3	A	1202	O31	F54-C41-F53	3.23	107.78	105.22
3	A	1202	O31	C55-C27-C25	-2.93	109.64	113.40
3	A	1202	O31	C11-C09-N08	-2.90	110.67	115.70
3	A	1202	O31	C12-C11-N17	-2.72	114.14	117.80
3	A	1202	O31	C12-C11-C13	2.43	60.37	59.12
3	A	1202	O31	C13-C11-N17	-2.35	111.21	117.62
3	A	1202	O31	O30-C29-N28	-2.24	121.17	124.85
3	A	1202	O31	C03-C02-C04	2.15	60.67	59.54
3	A	1202	O31	C11-C12-C13	-2.06	59.82	60.84
3	A	1202	O31	C42-N43-C44	2.03	119.23	115.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	O31	F53-C41-C42-N43
3	A	1202	O31	C09-N08-S05-C02
3	A	1202	O31	C39-C40-C41-F54

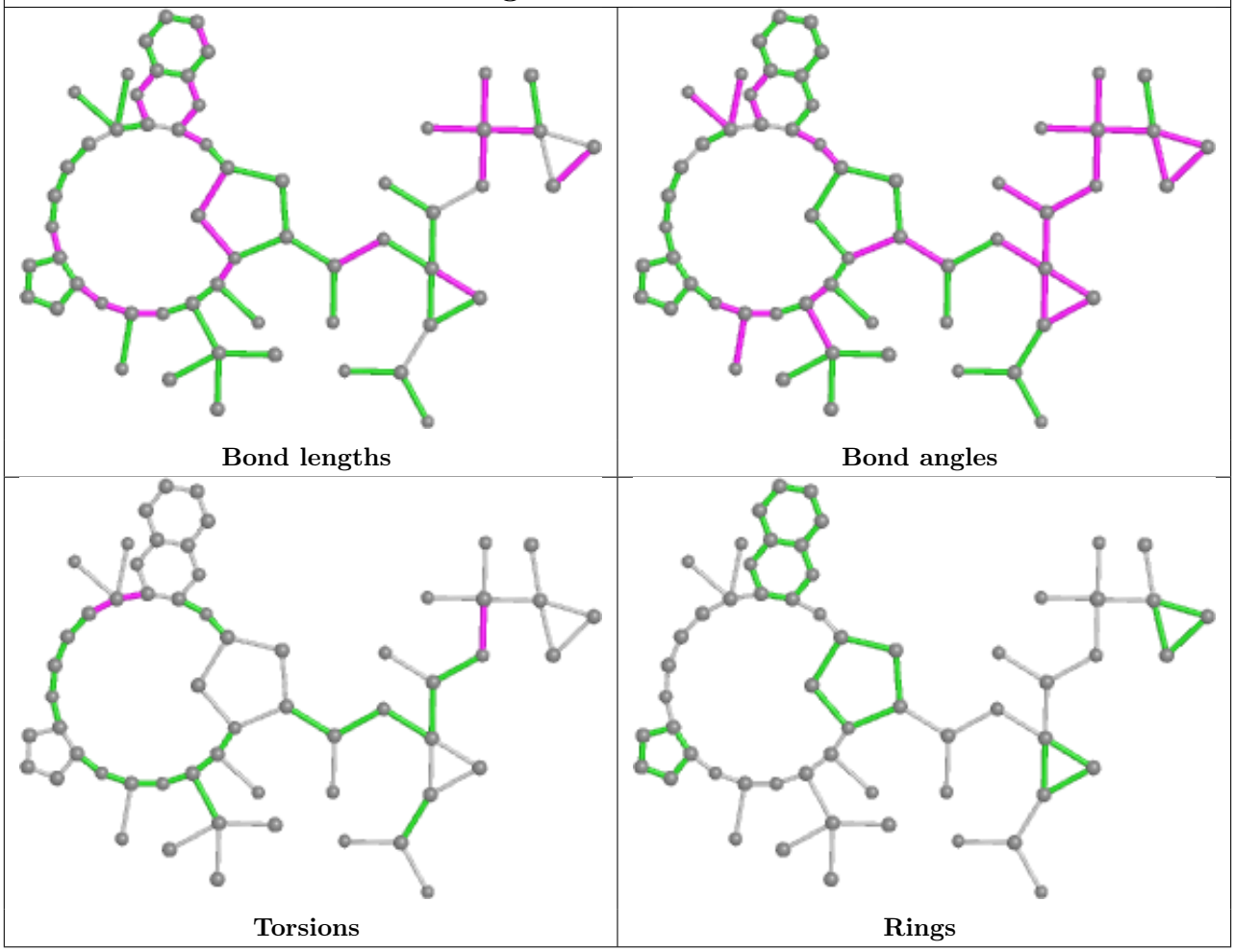
There are no ring outliers.

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.

Ligand O31 A 1202



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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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