



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:22 am BST

PDB ID : 1CQQ  
Title : TYPE 2 RHINOVIRUS 3C PROTEASE WITH AG7088 INHIBITOR  
Authors : Matthews, D.; Ferre, R.A.  
Deposited on : 1999-08-10  
Resolution : 1.85 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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.11

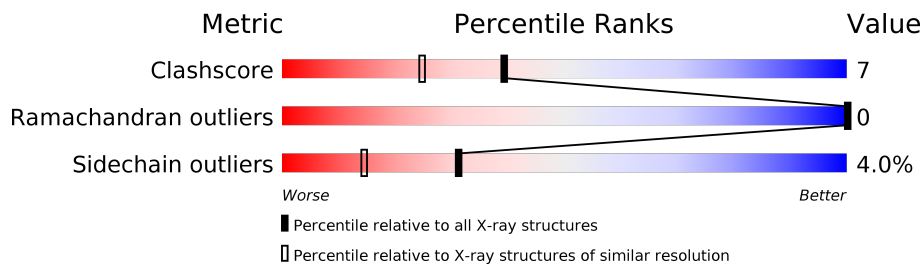
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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 on 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	180	

## 2 Entry composition [i](#)

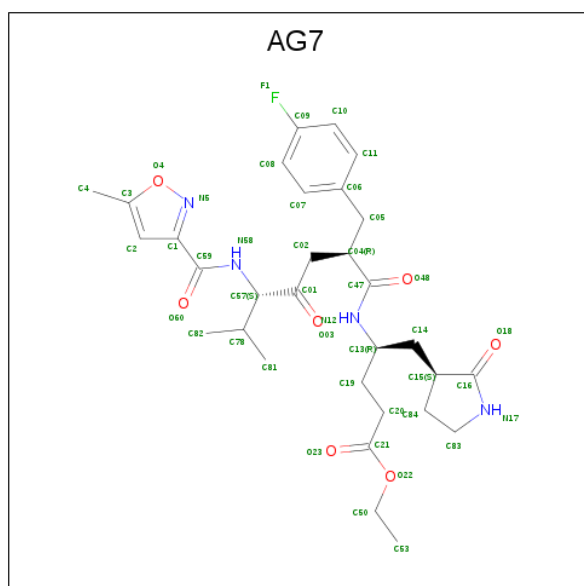
There are 3 unique types of molecules in this entry. The entry contains 2446 atoms, of which 792 are hydrogens and 0 are deuteriums.

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 TYPE 2 RHINOVIRUS 3C PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	180	1700	880	310	236	268	6	317	0	0

- Molecule 2 is 4-{2-(4-FLUORO-BENZYL)-6-METHYL-5-[(5-METHYL-ISOXAZOLE-3-CARBONYL)-AMINO]-4-OXO-HEPTANOYLAMINO}-5-(2-OXO-PYRROLIDIN-3-YL)-PENTANOIC ACID ETHYL ESTER (three-letter code: AG7) (formula: C<sub>31</sub>H<sub>41</sub>FN<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			O
2	A	1	83	31	1	40	4	7	40	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	H			O
3	A	221	663	442	221	442	0



## 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, $\alpha$ , $\beta$ , $\gamma$	34.30Å 65.70Å 77.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	87.1 (10.00-1.85)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AG7

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	1.04	0/1417	1.66	26/1921 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	89	TYR	CB-CG-CD2	-9.94	115.04	121.00
1	A	180	THR	CB-CA-C	9.22	136.49	111.60
1	A	88	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	A	33	ARG	NE-CZ-NH2	8.39	124.49	120.30
1	A	134	ARG	NE-CZ-NH2	8.31	124.45	120.30
1	A	180	THR	N-CA-C	-7.23	91.48	111.00
1	A	87	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	A	84	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	180	THR	N-CA-CB	-6.63	97.70	110.30
1	A	176	ARG	CD-NE-CZ	-6.38	114.67	123.60
1	A	178	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	A	87	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	96	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	A	88	ARG	CG-CD-NE	-5.92	99.36	111.80
1	A	94	GLU	CA-CB-CG	5.80	126.16	113.40
1	A	60	TYR	CB-CG-CD2	-5.72	117.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	A	167	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	A	147	CYS	CA-CB-SG	-5.62	103.88	114.00
1	A	42	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	37	VAL	CA-CB-CG1	-5.48	102.68	110.90
1	A	122	TYR	N-CA-CB	-5.29	101.07	110.60
1	A	33	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	A	76	LYS	CA-CB-CG	-5.11	102.16	113.40
1	A	92	ASN	CB-CA-C	-5.09	100.21	110.40
1	A	176	ARG	CA-CB-CG	-5.08	102.23	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	TYR	Sidechain

## 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	1390	310	1362	21	0
2	A	43	40	40	2	0
3	A	221	442	0	5	0
All	All	1654	792	1402	21	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 7.

All (21) 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:A:11:ILE:HG21	1:A:111:PRO:HB3	1.80	0.63
1:A:128:SER:HB3	3:A:817:HOH:O	2.00	0.61
1:A:19:THR:HB	1:A:48:GLN:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HG2	1:A:138:TYR:N	2.19	0.57
1:A:11:ILE:HA	1:A:15:SER:HB3	1.87	0.55
1:A:58:ASP:HB2	3:A:891:HOH:O	2.06	0.54
1:A:116:VAL:HA	1:A:140:TYR:CD1	2.45	0.52
1:A:48:GLN:HE21	1:A:51:GLY:HA2	1.74	0.52
1:A:25:PHE:CZ	1:A:41:ALA:HA	2.47	0.49
1:A:124:ASN:HD22	1:A:131:GLN:NE2	2.09	0.49
1:A:114:ILE:HD13	3:A:653:HOH:O	2.12	0.48
1:A:39:THR:HA	1:A:73:THR:OG1	2.15	0.46
1:A:18:ILE:HD12	1:A:47:ILE:HD12	1.97	0.45
1:A:125:ILE:HD11	1:A:127:LEU:HD13	1.98	0.45
1:A:125:ILE:HG12	1:A:135:MET:HG3	2.00	0.43
1:A:79:ARG:HD2	3:A:611:HOH:O	2.18	0.43
1:A:134:ARG:HG2	1:A:173:MET:CE	2.50	0.42
1:A:40:HIS:NE2	2:A:501:AG7:H42	2.35	0.41
1:A:147:CYS:HB2	2:A:501:AG7:C21	2.50	0.41
1:A:134:ARG:O	1:A:173:MET:HB2	2.21	0.41
1:A:144:SER:HB2	3:A:823:HOH:O	2.20	0.41

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	178/180 (99%)	169 (95%)	9 (5%)	0	<a href="#">100</a> <a href="#">100</a>

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	151/155 (97%)	145 (96%)	6 (4%)	31 14

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	58	ASP
1	A	75	LEU
1	A	79	ARG
1	A	110	GLU
1	A	138	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	131	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 carbohydrates in this entry.

## 5.6 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AG7	A	501	1	42,45,45	1.35	4 (9%)	49,61,61	1.49	10 (20%)

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	AG7	A	501	1	-	6/40/54/54	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AG7	C1-C59	-4.57	1.39	1.50
2	A	501	AG7	C4-C3	3.65	1.52	1.48
2	A	501	AG7	C16-N17	-3.41	1.30	1.33
2	A	501	AG7	C05-C06	-2.26	1.45	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AG7	C06-C05-C04	-3.37	107.54	113.72
2	A	501	AG7	C78-C57-N58	-3.29	103.29	111.43
2	A	501	AG7	C78-C57-C01	3.01	114.84	110.89
2	A	501	AG7	O60-C59-N58	-2.78	117.34	122.45
2	A	501	AG7	C1-C2-C3	-2.57	102.75	106.06
2	A	501	AG7	C82-C78-C57	2.52	118.29	111.16
2	A	501	AG7	C04-C47-N12	2.34	120.26	116.21
2	A	501	AG7	O48-C47-N12	-2.26	118.75	122.93
2	A	501	AG7	C84-C15-C16	-2.24	99.97	102.88
2	A	501	AG7	O18-C16-N17	-2.16	122.54	125.54

There are no chirality outliers.

All (6) torsion outliers are listed below:

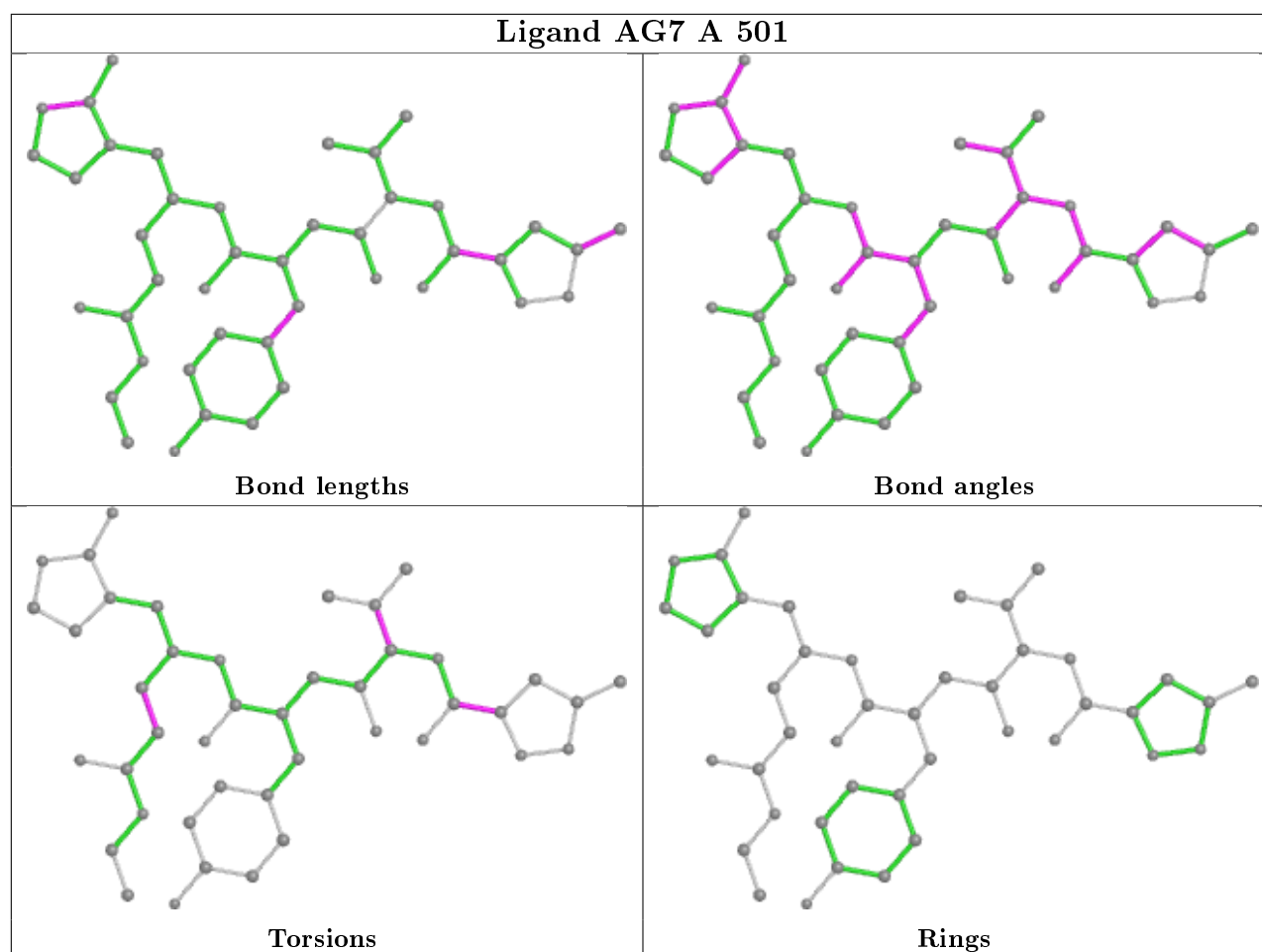
Mol	Chain	Res	Type	Atoms
2	A	501	AG7	C01-C57-C78-C82
2	A	501	AG7	N58-C57-C78-C81
2	A	501	AG7	N58-C57-C78-C82
2	A	501	AG7	C01-C57-C78-C81
2	A	501	AG7	C13-C19-C20-C21
2	A	501	AG7	C2-C1-C59-O60

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AG7	2	0

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 than 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.



## 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.