

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

#### Apr 18, 2024 – 01:22 PM EDT

PDB ID	:	7H3E
Title	:	Group deposition for crystallographic fragment screening of Coxsackievirus
		A16 (G-10) 2A protease – Crystal structure of Coxsackievirus A16 (G-10) 2A
		protease in complex with Z56921372 (A71EV2A-x0375)
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		X.; Thompson, W.; Tomlinson, C.W.E.; Wild, C.; Winokan, M.; Xavier, M
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Deposited on	:	2024-04-04
Resolution	:	1.39 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:

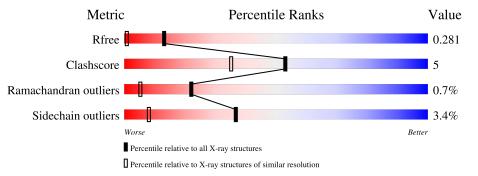
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

# 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 1.39 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain	
1	А	150	81%	11% • 7%



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1363 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.

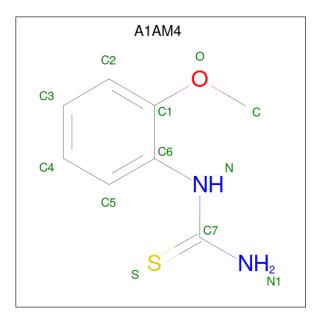
• Molecule 1 is a protein called Protease 2A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	140	Total 1103	C 686	N 196	0 214	${f S}7$	0	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLN	-	expression tag	UNP Q65900
А	2	GLU	-	expression tag	UNP Q65900
A	3	GLN	-	expression tag	UNP Q65900
А	4	THR	-	expression tag	UNP Q65900
А	5	GLY	-	expression tag	UNP Q65900
А	6	GLY	-	expression tag	UNP Q65900

• Molecule 2 is N-(2-methoxyphenyl)thiourea (three-letter code: A1AM4) (formula:  $C_8H_{10}N_2OS$ ).



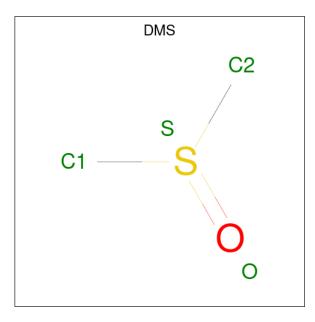


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Δ	1	Total	С	Ν	0	S	0	0
2	Л	1	12	8	2	1	1	0	0
2	٨	A 1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
	Z A		12	8	2	1	1	0	0
2	Λ	1	Total	С	Ν	0	S	0	0
	Л	1	12	8	2	1	1	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

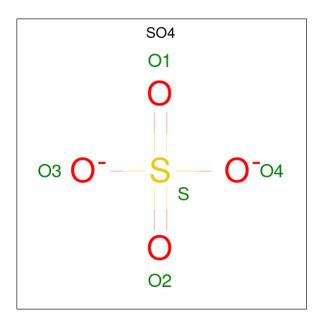
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Zn 1 1	0	0

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0





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

• Molecule 6 is water.

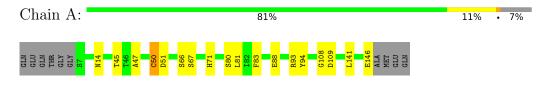
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	206	Total         O           206         206	0	0



# 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.

• Molecule 1: Protease 2A





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	85.92Å 56.73Å 32.42Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $94.69^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	32.33 - 1.39	Depositor
Resolution (A)	32.31 - 1.39	EDS
% Data completeness	98.3 (32.33-1.39)	Depositor
(in resolution range)	98.3 (32.31-1.39)	EDS
R <sub>merge</sub>	0.08	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.18 (at 1.39 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
D D	0.201 , 0.246	Depositor
$R, R_{free}$	0.248 , $0.281$	DCC
$R_{free}$ test set	1550 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	19.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.28, 36.4	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1363	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.25% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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.

## 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: A1AM4, DMS, ZN, SO4  $\,$ 

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	А	0.78	0/1129	0.90	1/1535~(0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	50	CYS	CB-CA-C	-5.04	100.31	110.40

There are no chirality outliers.

There are no planarity outliers.

### 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	А	1103	0	1034	12	0
2	А	36	0	0	0	0
3	А	1	0	0	0	0
4	А	12	0	18	0	0
5	А	5	0	0	0	0
6	А	206	0	0	7	0
All	All	1363	0	1052	12	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 5.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:O	6:A:301:HOH:O	2.12	0.67
1:A:141:LEU:HG	6:A:352:HOH:O	1.97	0.63
1:A:81:LEU:HG	1:A:94:TYR:HB3	1.85	0.58
1:A:14:ASN:HA	1:A:45:THR:OG1	2.07	0.55
1:A:50:CYS:C	6:A:315:HOH:O	2.48	0.51
1:A:71:HIS:HE1	6:A:399:HOH:O	1.94	0.50
1:A:50:CYS:HB2	6:A:448:HOH:O	2.14	0.47
1:A:66:SER:OG	1:A:109:ASP:OD1	2.17	0.44
1:A:67:SER:N	1:A:109:ASP:OD1	2.51	0.43
1:A:51:ASP:N	6:A:315:HOH:O	2.53	0.41
1:A:81:LEU:CG	1:A:94:TYR:HB3	2.51	0.40
1:A:47:ALA:HB3	6:A:401:HOH:O	2.21	0.40

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	А	141/150~(94%)	137~(97%)	3~(2%)	1 (1%)	22 5

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	А	83	PHE	

#### 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	Analysed Rotameric		Percentiles	
1	А	120/124~(97%)	115 (96%)	5(4%)	30 5	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	80[A]	SER
1	А	80[B]	SER
1	А	88	GLU
1	А	93	ARG
1	А	146	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type	
1	А	71	HIS	

#### 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)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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



Mol	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
5	SO4	А	208	-	$4,\!4,\!4$	0.35	0	$6,\!6,\!6$	0.06	0
2	A1AM4	А	203	-	12,12,12	0.16	0	$15,\!15,\!15$	0.34	0
4	DMS	А	207	-	$3,\!3,\!3$	0.29	0	$3,\!3,\!3$	0.16	0
4	DMS	А	206	-	$3,\!3,\!3$	0.24	0	$3,\!3,\!3$	0.13	0
2	A1AM4	А	202	-	$12,\!12,\!12$	0.26	0	$15,\!15,\!15$	0.50	0
2	A1AM4	А	201	-	12,12,12	0.28	0	$15,\!15,\!15$	0.33	0
4	DMS	А	205	-	3,3,3	0.35	0	$3,\!3,\!3$	0.07	0

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).

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	A1AM4	А	201	-	-	0/6/6/6	0/1/1/1
2	A1AM4	А	202	-	-	3/6/6/6	0/1/1/1
2	A1AM4	А	203	-	-	3/6/6/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	202	A1AM4	С6-С1-О-С
2	А	202	A1AM4	С2-С1-О-С
2	А	203	A1AM4	С6-С1-О-С
2	А	203	A1AM4	С2-С1-О-С
2	А	203	A1AM4	C1-C6-N-C7
2	А	202	A1AM4	C1-C6-N-C7

There are no ring outliers.

No monomer is involved in short contacts.

### 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 (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

