

Full wwPDB X-ray Structure Validation Report (i)

Apr 18, 2024 – 01:32 PM EDT

PDB ID	:	7H54
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 Z57473948 (A71EV2A-x1292)
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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	:	1.10 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:

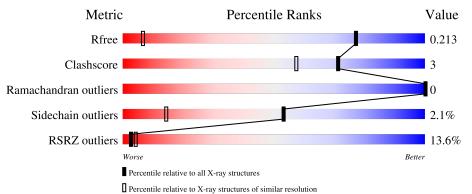
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.10 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain					
1	А	150	5% 89%	•• 7%				
1	В	150	86%	7% • 7%				

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996) Validation Pipeline (wwPDB-VP) : 2.36.1



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	T7U	В	201	-	-	-	Х



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2630 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	1 A	140	Total	С	Ν	0	S	0	3	0
		140	1101	685	196	213	$\overline{7}$	0		
1	В	140	Total	С	Ν	0	S	0	2	0
	В	140	1103	688	196	212	7	0	3	0

• Molecule 1 is a protein called Protease 2A.

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

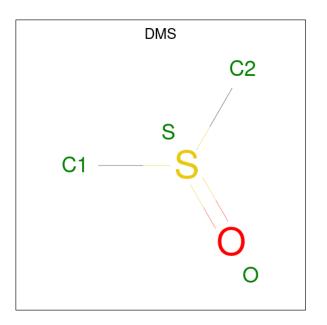
There are 12 discrepancies between the modelled and reference sequences:

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0

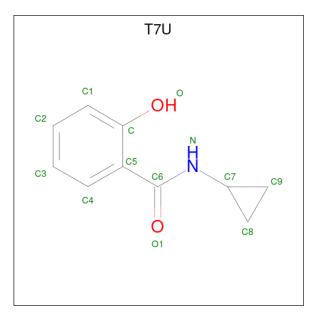
• Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 4	${ m C} 2$		S 1	0	0
3	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

• Molecule 4 is N-cyclopropyl-2-hydroxybenzamide (three-letter code: T7U) (formula: $C_{10}H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total 13	C 10	N 1	O 2	0	0



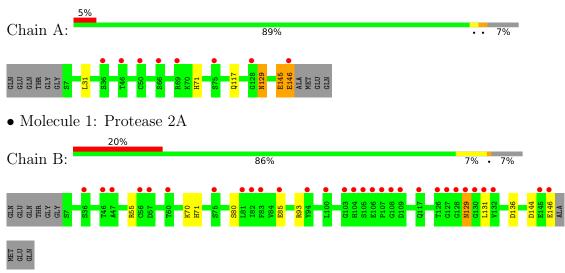
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	204	Total O 204 204	0	0
5	В	199	Total O 199 199	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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	86.07Å 56.60Å 64.48Å	Depositor
a, b, c, α , β , γ	90.00° 94.68° 90.00°	Depositor
Resolution (Å)	42.93 - 1.10	Depositor
Resolution (A)	42.89 - 1.10	EDS
% Data completeness	94.2 (42.93-1.10)	Depositor
(in resolution range)	94.3 (42.89-1.10)	EDS
R _{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 1.10 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
D D.	0.175 , 0.194	Depositor
R, R_{free}	0.194 , 0.213	DCC
R_{free} test set	5354 reflections $(4.50%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	13.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 38.1	EDS
L-test for twinning ²	$ L > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2630	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 67.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0528e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities 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: DMS, T7U, ZN $\,$

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).

Mal	Mol Chain		lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.82	0/1127	0.91	0/1532	
1	В	0.79	0/1129	0.88	2/1535~(0.1%)	
All	All	0.81	0/2256	0.90	2/3067~(0.1%)	

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	А	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	93	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	В	136	ASP	CB-CG-OD2	-5.85	113.04	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	145	GLU	Peptide

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1101	0	1035	8	0
1	В	1103	0	1041	7	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	8	0	12	1	0
4	В	13	0	0	0	0
5	А	204	0	0	4	0
5	В	199	0	0	2	0
All	All	2630	0	2088	15	0

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.

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 3.

All (15) 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:85:GLU:HG2	5:B:448:HOH:O	1.88	0.73
1:A:146:GLU:HG3	1:A:146:GLU:O	1.95	0.67
1:B:129:ASN:HD21	1:B:131:LEU:HD12	1.61	0.66
1:A:146:GLU:O	1:A:146:GLU:CG	2.50	0.60
1:B:70:LYS:HE3	5:B:360:HOH:O	2.06	0.56
1:A:71:HIS:HD2	5:A:466:HOH:O	1.93	0.50
1:B:129:ASN:HD21	1:B:131:LEU:CD1	2.25	0.49
1:A:117:GLN:HG2	5:A:384:HOH:O	2.13	0.48
1:B:55:ARG:HH21	1:B:144:ASP:CG	2.16	0.48
1:A:71:HIS:HE1	5:A:433:HOH:O	1.99	0.45
3:A:203:DMS:H23	5:A:433:HOH:O	2.18	0.44
1:A:129:ASN:HD22	1:A:129:ASN:HA	1.75	0.43
1:B:129:ASN:O	1:B:129:ASN:ND2	2.45	0.43
1:A:145:GLU:HG3	1:A:146:GLU:HB3	2.02	0.41
1:A:31:LEU:HD23	1:B:71:HIS:CD2	2.56	0.40

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	Perce	ntiles
1	А	141/150~(94%)	139 (99%)	2(1%)	0	100	100
1	В	141/150~(94%)	139~(99%)	2(1%)	0	100	100
All	All	282/300~(94%)	278~(99%)	4 (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	Percer	ntiles
1	А	120/124~(97%)	118 (98%)	2(2%)	60	23
1	В	120/124~(97%)	117~(98%)	3~(2%)	47	10
All	All	240/248~(97%)	235~(98%)	5(2%)	53	14

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

Mol	Chain	Res	Type
1	А	129	ASN
1	А	146	GLU
1	В	80	SER
1	В	129	ASN
1	В	146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	14	ASN
1	А	48	GLN
1	А	71	HIS
1	А	129	ASN
1	В	14	ASN
1	В	71	HIS
1	В	129	ASN

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	Trune	Chain	Dec	Dec	Dog	Dec	Dec	Res	Dog	Dec	Dog	Dec	Dec	Dec	Link	Bo	Bond lengths			ond ang	les
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2											
3	DMS	А	202	-	3,3,3	0.36	0	3,3,3	0.11	0											
4	T7U	В	201	-	14,14,14	0.19	0	19,19,19	0.41	0											
3	DMS	А	203	-	3,3,3	0.19	0	3,3,3	0.13	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.



Μ	ol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4		T7U	В	201	-	-	1/8/10/10	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	201	T7U	C-C5-C6-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	203	DMS	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	$\#RSRZ{>}2$	$\mathbf{OWAB}(\mathbf{A}^2)$	$Q{<}0.9$
1	А	140/150~(93%)	0.38	8 (5%) 23 22	9, 13, 24, 46	4(2%)
1	В	140/150~(93%)	1.46	30 (21%) 0 2	9,13,25,57	24 (17%)
All	All	280/300~(93%)	0.92	38 (13%) 3 4	9,13,25,57	28 (10%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	82	ILE	14.2	
1	В	100[A]	LEU	13.7	
1	В	56	CYS	12.9	
1	В	132	VAL	10.9	
1	В	81	LEU	9.7	
1	В	131	LEU	9.4	
1	А	75[A]	SER	9.0	
1	В	83	PHE	8.5	
1	В	60	THR	8.2	
1	В	103	GLY	7.5	
1	В	36[A]	SER	7.4	
1	В	57	ASP	7.1	
1	В	105	SER	6.8	
1	А	66[A]	SER	6.8	
1	В	126	THR	6.7	
1	В	127	GLY	6.7	
1	В	75[A]	SER	6.5	
1	А	36[A]	SER	6.3	
1	В	108	GLY	5.9	
1	В	104	HIS	5.8	
1	В	130	GLY	5.6	
1	А	69	ARG	5.3	
1	В	109	ASP	5.2	
1	В	107	PRO	4.9	

Continued on next page...



Mol	nuea fron Chain	Res	Type	RSRZ
1	В	146	GLU	4.6
1	В	129	ASN	4.5
1	В	128	GLY	4.5
1	В	106	GLU	3.8
1	В	145	GLU	3.6
1	А	128	GLY	3.5
1	А	146	GLU	3.5
1	В	46	THR	3.2
1	В	94	TYR	3.1
1	В	85	GLU	3.0
1	В	117	GLN	2.6
1	А	50	CYS	2.5
1	А	46	THR	2.4
1	В	47	ALA	2.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	T7U	В	201	13/13	0.30	0.42	$30,\!34,\!42,\!42$	13
3	DMS	А	203	4/4	0.72	0.17	72,78,79,79	0
3	DMS	А	202	4/4	0.84	0.32	$29,\!47,\!54,\!58$	0
2	ZN	В	202	1/1	0.95	0.08	$15,\!15,\!15,\!15$	0
2	ZN	А	201	1/1	0.99	0.05	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.

