

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

### May 15, 2020 – 08:19 pm BST

:	6SEL
:	Multicrystal structure of Thermolysin at room temperature using a multilayer
	monochromator.
:	Sandy, J.; Sanchez-Weatherby, J.; Mikolajek, H.
:	2019-07-30
:	2.20  Å(reported)
	:

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

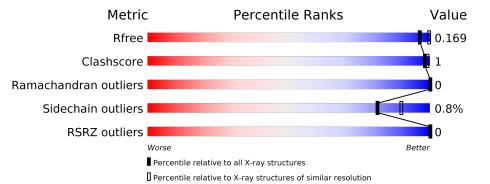
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	4898 (2.20-2.20)
Clashscore	141614	5594(2.20-2.20)
Ramachandran outliers	138981	5503(2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 >=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	316	98% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	$\mathbf{Res}$	Chirality	Geometry	Clashes	Electron density
5	CA	А	407	-	-	-	Х



#### 6SEL

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5061 atoms, of which 2336 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.

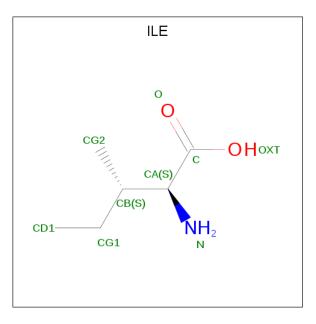
• Molecule 1 is a protein called Thermolysin.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	316	Total 4825	C 1572	Н 2333	N 419	O 499	${ m S} 2$	1	14	0

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

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

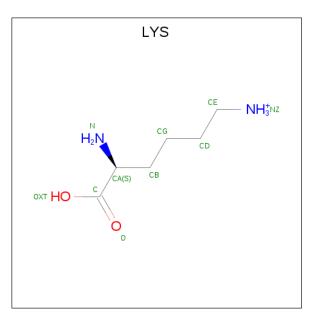
• Molecule 3 is ISOLEUCINE (three-letter code: ILE) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
3	А	1	Total 9	$\begin{array}{c} \mathrm{C} \\ \mathrm{6} \end{array}$	Н 1	N 1	0 1	1	0

• Molecule 4 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
4	Δ	1	Total	С	Η	Ν	Ο	0	0
4	А	1	12	6	2	2	2	2	0

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	5	Total Ca 5 5	0	0

• Molecule 6 is water.

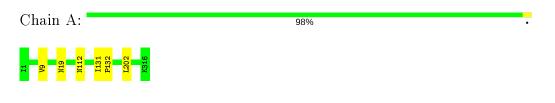
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	209	Total         O           209         209	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Thermolysin





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	93.56Å $93.56$ Å $130.59$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	81.02 - 2.20	Depositor
Resolution (A)	81.02 - 2.20	EDS
% Data completeness	$100.0 \ (81.02-2.20)$	Depositor
(in resolution range)	$96.6\ (81.02-2.20)$	EDS
R <sub>merge</sub>	0.13	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.93 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
$R, R_{free}$	0.129 , $0.169$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.130 , $0.169$	DCC
$R_{free}$ test set	1777 reflections $(9.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	22.6	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36 , $36.0$	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	0.97	EDS
Total number of atoms	5061	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 3.93% 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: ZN, CA

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	
	101	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
	1	А	0.45	0/2601	0.61	1/3542~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	202	LEU	CA-CB-CG	5.03	126.87	115.30

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	2492	2333	2356	3	0
2	А	1	0	0	0	0
3	А	8	1	10	0	0
4	А	10	2	13	0	0
5	А	5	0	0	0	0
6	А	209	0	0	0	0
All	All	2725	2336	2379	3	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 1.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:131:ILE:HB	1:A:132:PRO:CD	2.44	0.47	
1:A:131:ILE:HB	1:A:132:PRO:HD2	1.96	0.46	
1:A:9[B]:VAL:HG22	1:A:19:ASN:OD1	2.19	0.43	

All (3) 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		
1	А	327/316~(104%)	317~(97%)	10 (3%)	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.

N	Mol	Chain	Analysed	Analysed Rotameric		Percentiles	
	1	А	266/252~(106%)	265~(100%)	1 (0%)	91 96	

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	112	ASN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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)

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<sup>th</sup> 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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	316/316~(100%)	-0.73	0 100 100	14, 23, 35, 64	0

There are no RSRZ outliers to report.

## 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 carbohydrates 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
5	CA	А	407	1/1	0.78	0.56	$85,\!85,\!85,\!85$	0
4	LYS	А	403	10/10	0.91	0.13	$31,\!37,\!44,\!47$	2
3	ILE	А	402	8/9	0.98	0.10	$20,\!25,\!30,\!32$	1
5	CA	А	408	1/1	0.99	0.06	$28,\!28,\!28,\!28$	0
5	CA	А	404	1/1	0.99	0.08	$20,\!20,\!20,\!20$	0
5	CA	А	406	1/1	1.00	0.08	$19,\!19,\!19,\!19$	0
2	ZN	А	401	1/1	1.00	0.11	$18,\!18,\!18,\!18$	0
5	CA	А	405	1/1	1.00	0.05	$29,\!29,\!29,\!29$	0



## 6.5 Other polymers (i)

There are no such residues in this entry.

