

wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2022 – 03:32 PM EST

PDB ID : 2TMN

Title : CRYSTALLOGRAPHIC STRUCTURAL ANALYSIS OF PHOSPHORAMI-

DATES AS INHIBITORS AND TRANSITION-STATE ANALOGS OF

THERMOLYSIN

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Deposited on : 1987-06-29

Resolution : 1.60 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 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.31.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

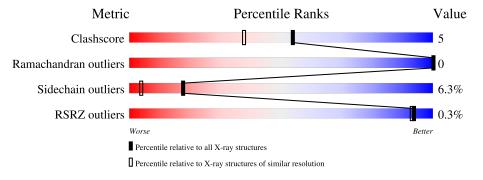
Validation Pipeline (wwPDB-VP) : 2.31.2

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 1.60 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 $(\#\text{Entries, resolution range}(\mathring{A}))$
Clashscore	141614	3665 (1.60-1.60)
	141014	,
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	Е	316	67%	25%	7% •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2618 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 Thermolysin.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Е	316	Total 2432	C 1528	N 408	O 494	S 2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	n Residue Modelled		Actual	Comment	Reference	
Е	37	ASP	ASN	conflict	UNP P00800	
Е	119	GLU	GLN	conflict	UNP P00800	

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

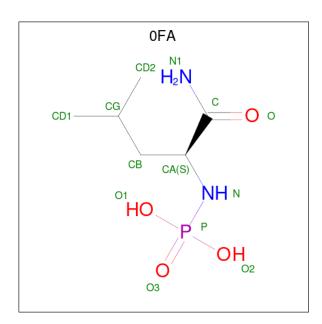
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Е	4	Total Ca 4 4	0	0

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

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

• Molecule 4 is N 2 -phosphono-L-leucinamide (three-letter code: 0FA) (formula: $C_6H_{15}N_2O_4P$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
4	E	1	Total	С	N	O	P	0	0
			13	6	2	4	Ţ		

• Molecule 5 is water.

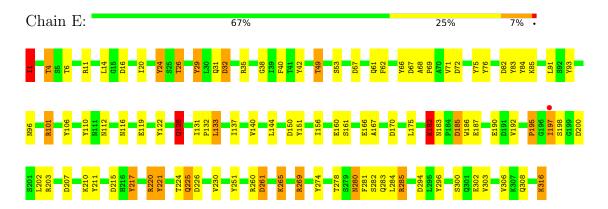
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	168	Total O 168 168	0	0



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: Thermolysin





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 61 2 2	Depositor	
Cell constants	94.10Å 94.10Å 131.40Å	Donositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	(Not available) – 1.60	Depositor	
Resolution (A)	29.83 - 1.60	EDS	
% Data completeness	(Not available) ((Not available)-1.60)	Depositor	
(in resolution range)	69.2 (29.83-1.60)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	0.28 (at 1.60Å)	Xtriage	
Refinement program	TNT	Depositor	
D D.	0.179 , (Not available)	Depositor	
R, R_{free}	0.163 , (Not available)	DCC	
R_{free} test set	No test flags present.	wwPDB-VP	
Wilson B-factor (Å ²)	14.5	Xtriage	
Anisotropy	0.621	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.32\;,63.2$	EDS	
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.34$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.97	EDS	
Total number of atoms	2618	wwPDB-VP	
Average B, all atoms (Å ²)	16.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: ZN, 0FA, 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	Bo	nd lengths	В	ond angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	Е	1.34	$10/2491 \ (0.4\%)$	2.06	107/3391 (3.2%)

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	2	0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	Е	166	GLU	CD-OE2	7.93	1.34	1.25
1	Е	187	GLU	CD-OE2	7.71	1.34	1.25
1	Е	160	GLU	CD-OE1	-7.57	1.17	1.25
1	Е	166	GLU	CD-OE1	-6.79	1.18	1.25
1	Е	316	LYS	C-OXT	6.07	1.34	1.23

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	Е	35	ARG	NE-CZ-NH1	13.95	127.27	120.30
1	Е	220	ARG	NE-CZ-NH2	-13.05	113.78	120.30
1	Е	269	ARG	NE-CZ-NH1	-12.65	113.97	120.30
1	Е	274	TYR	CB-CG-CD1	-11.40	114.16	121.00
1	Е	260	ARG	NE-CZ-NH2	-11.28	114.66	120.30

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	Е	224	THR	СВ
1	Е	260	ARG	CA

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	Е	2432	0	2267	25	0
2	Е	4	0	0	0	0
3	Е	1	0	0	0	0
4	Е	13	0	13	0	0
5	Е	168	0	0	3	1
All	All	2618	0	2280	25	1

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.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:E:269:ARG:NH1	1:E:294:ASP:OD2	2.00	0.94
1:E:285:ARG:HD3	1:E:316:LYS:HD3	1.48	0.93
1:E:116:ASN:O	5:E:326:HOH:O	1.94	0.84
1:E:137:ILE:H	1:E:182:LYS:HZ2	1.43	0.66
1:E:265:LYS:HE2	5:E:411:HOH:O	1.95	0.64

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
5:E:441:HOH:O	5:E:441:HOH:O[7_555]	1.41	0.79



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	E	314/316 (99%)	303 (96%)	11 (4%)	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	Percentiles		
1	Е	252/252 (100%)	236 (94%)	16 (6%)	18 4		

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	265	LYS
1	Е	261	ASP
1	Е	183	ASN
1	Е	225	GLN
1	Е	182	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	31	GLN
1	Е	33	ASN
1	Е	97	ASN

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Mol	Chain	Res	Type
1	E	280	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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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		$\operatorname{A} = \operatorname{A} = $		Bo	Bond lengths			Bond angles		
	IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	4	0FA	Е	322	3	12,12,12	6.35	2 (16%)	15,17,17	1.71	3 (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
4	0FA	Е	322	3	-	2/11/13/13	-

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	E	322	0FA	P-N	21.77	1.85	1.61
4	Е	322	0FA	P-O3	2.25	1.49	1.46

All (3) bond angle outliers are listed below:

ľ	Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
	4	Е	322	0FA	O3-P-N	-3.61	106.85	113.04
	4	Е	322	0FA	CD2-CG-CB	-3.40	98.60	111.11
	4	Е	322	0FA	O-C-CA	-2.63	116.42	120.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	322	0FA	N1-C-CA-N
4	Е	322	0FA	CA-N-P-O3

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^{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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	Е	316/316 (100%)	-0.80	1 (0%) 94 93	7, 14, 28, 37	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	197	ILE	2.3

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	CA	Ε	320	1/1	0.99	0.03	16,16,16,16	0
4	0FA	Е	322	13/13	0.99	0.06	10,14,17,17	0
2	CA	Ε	319	1/1	1.00	0.03	12,12,12,12	0
2	CA	Ε	317	1/1	1.00	0.04	11,11,11,11	0
3	ZN	Ε	321	1/1	1.00	0.03	11,11,11,11	0
2	CA	Ε	318	1/1	1.00	0.03	13,13,13,13	0



6.5 Other polymers (i)

There are no such residues in this entry.

