

Full wwPDB X-ray Structure Validation Report (i)

Jan 29, 2024 – 08:41 PM EST

PDB ID : 1FJV

Title: THERMOLYSIN (60% ACETONITRILE SOAKED CRYSTALS)

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Deposited on : 2000-08-08

Resolution : 2.00 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

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

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

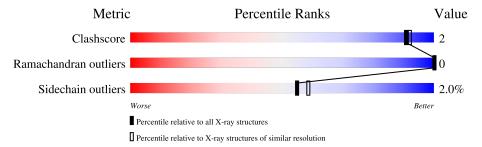
Validation Pipeline (wwPDB-VP) : 2.36

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 2.00 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	316	88%	11%	•



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2639 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	A	316	Total 2454	C 1540	N 415	O 497	S 2	0	5	0

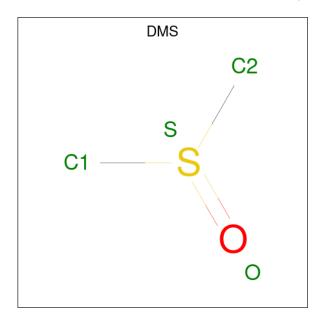
• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Ca 4 4	0	0

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C O 2 1	S 1	0	0

$\bullet\,$ Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	176	Total O 176 176	0	0

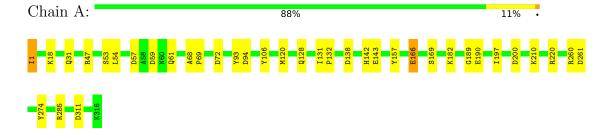


3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: THERMOLYSIN





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 61 2 2	Depositor	
Cell constants	93.97Å 93.97Å 131.12Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	20.00 - 2.00	Depositor	
% Data completeness	96.0 (20.00-2.00)	Depositor	
(in resolution range)	30.0 (20.00-2.00)	Depositor	
R_{merge}	0.10	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC	Depositor	
R, R_{free}	0.153 , 0.206	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2639	wwPDB-VP	
Average B, all atoms (Å ²)	25.0	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: ZN, CA, DMS

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	Chain	Bo	nd lengths	Во	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.68	$1/2540 \ (0.0\%)$	1.43	$22/3456 \ (0.6\%)$

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
1	A	53	SER	CA-CB	5.00	1.60	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
1	A	166	GLU	OE1-CD-OE2	-18.91	100.61	123.30
1	A	200	ASP	CB-CG-OD2	15.80	132.52	118.30
1	A	190	GLU	OE1-CD-OE2	-10.54	110.65	123.30
1	A	57	ASP	CB-CG-OD2	10.41	127.67	118.30
1	A	59	ASP	CB-CG-OD2	10.34	127.61	118.30
1	A	166	GLU	CG-CD-OE2	8.51	135.33	118.30
1	A	47	ARG	CD-NE-CZ	8.20	135.09	123.60
1	A	200	ASP	CB-CG-OD1	-8.05	111.05	118.30
1	A	220	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	197	ILE	CA-C-N	7.25	133.14	117.20
1	A	138	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	261	ASP	CB-CG-OD1	6.35	124.02	118.30

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	A	285	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	106	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	93	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	47	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	311	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	61	GLN	CA-C-N	5.36	128.99	117.20
1	A	260	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	94	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	72	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	274	TYR	CB-CG-CD2	5.10	124.06	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	GLY	Mainchain

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	2454	0	2290	8	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	4	0	6	0	0
5	A	176	0	0	0	0
All	All	2639	0	2296	8	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 2.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:157[A]:TYR:OH	1:A:166:GLU:OE2	2.06	0.67

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:1:ILE:N	1:A:31:GLN:HE22	1.96	0.63
1:A:120:MET:SD	1:A:143:GLU:HB3	2.50	0.50
1:A:68:ALA:HB3	1:A:69:PRO:HD3	1.99	0.45
1:A:1:ILE:H3	1:A:31:GLN:HE22	1.64	0.44
1:A:1:ILE:HD12	1:A:54:LEU:HD23	1.99	0.43
1:A:131:ILE:HB	1:A:132:PRO:HD2	2.03	0.41
1:A:142:HIS:CG	1:A:169:SER:HB3	2.55	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	Percentiles	5
1	A	319/316 (101%)	309 (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.

\mathbf{Mol}	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	A	257/252 (102%)	252 (98%)	5 (2%)	57 61		

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



Mol	Chain	Res	Type
1	A	1	ILE
1	A	18	LYS
1	A	128	GLN
1	A	182	LYS
1	A	210	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	33	ASN
1	A	97	ASN
1	A	290	GLN
1	A	308	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 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	Dec	Link	В	ond leng	gths	В	ond ang	gles
MIOI			Chain Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	DMS	A	506	-	3,3,3	0.68	0	3,3,3	0.59	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

