

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

#### Mar 22, 2023 – 03:18 pm GMT

:	7ZAS
:	Crystal structure of cleaved Iripin-4 serpin from tick Ixodes ricinus
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	2022-03-22
:	2.00  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:

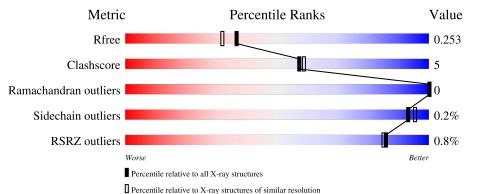
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

# 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 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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% 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	341	.% 89%	11%
1	В	341	% <b>8</b> 9%	11%
1	С	341	88%	11%
1	D	341	% 93%	7%
2	aa	35	91%	9%



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Mol	Chain	Length	Quality of chain	
2	bb	35	94% 69	%
2	сс	35	3% 97%	•
2	dd	35	91% 9%	_



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13196 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	Δ	341	Total	С	Ν	Ο	S	0	4	0
	А	341	2684	1709	459	510	6	0	4	0
1	В	341	Total	С	Ν	0	S	0	4	0
	D	041	2685	1710	460	509	6	0		
1	С	341	Total	С	Ν	0	S	0	5	0
	U	041	2695	1717	461	511	6	0	Э	0
1	Л	341	Total	С	Ν	0	S	0	1	0
	I D	341	2687	1712	460	509	6		4	0

• Molecule 1 is a protein called Iripin-4 serpin.

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	78	GLN	HIS	variant	UNP A0A0K8RJV9
А	155	GLU	GLY	variant	UNP A0A0K8RJV9
А	307	ASP	GLY	variant	UNP A0A0K8RJV9
В	78	GLN	HIS	variant	UNP A0A0K8RJV9
В	155	GLU	GLY	variant	UNP A0A0K8RJV9
В	307	ASP	GLY	variant	UNP A0A0K8RJV9
С	78	GLN	HIS	variant	UNP A0A0K8RJV9
С	155	GLU	GLY	variant	UNP A0A0K8RJV9
С	307	ASP	GLY	variant	UNP A0A0K8RJV9
D	78	GLN	HIS	variant	UNP A0A0K8RJV9
D	155	GLU	GLY	variant	UNP A0A0K8RJV9
D	307	ASP	GLY	variant	UNP A0A0K8RJV9

• Molecule 2 is a protein called Iripin-4 serpin.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	aa	32	Total	С	Ν	0	0	0	0
	aa	52	274	179	47	48	0	0	0
0	bb	33	Total	С	Ν	0	0	0	0
	00	55	281	184	48	49	0		0



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Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
0	cc 34	Total	С	Ν	0	0	0	0	
	сс	-04	289	190	49	50	0	0	0
0	44	32	Total	С	Ν	0	0	0	0
	dd	32	274	179	47	48	0	U	U

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cl 1 1	0	0
3	В	1	Total Cl 1 1	0	0
3	С	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

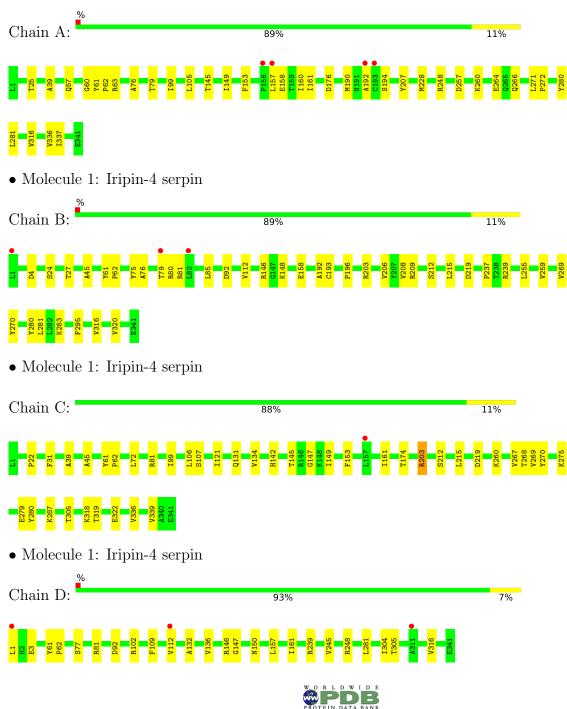
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	287	Total O 300 300	0	14
4	aa	22	TotalO2323	0	1
4	В	291	Total O 299 299	0	9
4	bb	25	Total O 27 27	0	2
4	С	324	Total O 330 330	0	8
4	сс	31	$\begin{array}{cc} \text{Total} & \text{O} \\ 31 & 31 \end{array}$	0	0
4	D	272	Total O 288 288	0	18
4	dd	24	Total O 25 25	0	1



## 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: Iripin-4 serpin

• Molecule 2: Iripin-4 serpin		
Chain aa:	91%	9%
SER VAL L376 L376		
• Molecule 2: Iripin-4 serpin		
Chain bb:	94%	6%
SER 1450 1376 1376		
• Molecule 2: Iripin-4 serpin		
Chain cc:	97%	·
SER 1.1376		
• Molecule 2: Iripin-4 serpin		
Chain dd:	91%	9%
SER VAEU VAEU L345 L376		



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	65.70Å 138.41Å 80.22Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $107.70^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	46.42 - 2.00	Depositor
Resolution (A)	46.42 - 2.00	EDS
% Data completeness	99.4 (46.42-2.00)	Depositor
(in resolution range)	$99.4 \ (46.42 - 2.00)$	EDS
R <sub>merge</sub>	(Not available) Deposite	
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.187 , $0.250$	Depositor
$R, R_{free}$	0.193 , $0.253$	DCC
$R_{free}$ test set	2100 reflections $(2.29%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	23.0	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , $43.7$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13196	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	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 45.37 % 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 1.3342e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: CL

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	
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.70	0/2745	0.81	0/3721
1	В	0.68	0/2743	0.81	0/3719
1	С	0.69	0/2753	0.82	0/3733
1	D	0.67	0/2748	0.79	0/3724
2	aa	0.63	0/281	0.83	0/378
2	bb	0.61	0/288	0.78	0/388
2	сс	0.65	0/296	0.81	0/399
2	dd	0.61	0/281	0.80	0/378
All	All	0.68	0/12135	0.81	0/16440

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
1	В	0	1
1	С	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

1A280TYRPeptide1B280TYRPeptide	Mol	Chain	Res	Type	Group
1 B 280 TYR Peptide	1	А	280	TYR	Peptide
	1	В	280	TYR	Peptide



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Mol	Chain	Res	Type	Group
1	С	280	TYR	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 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	2684	0	2705	30	0
1	В	2685	0	2707	26	0
1	С	2695	0	2716	28	0
1	D	2687	0	2713	16	0
2	aa	274	0	265	0	0
2	bb	281	0	274	0	0
2	сс	289	0	285	0	0
2	dd	274	0	265	0	0
3	А	1	0	0	1	0
3	В	1	0	0	1	0
3	С	1	0	0	1	0
3	D	1	0	0	1	0
4	А	300	0	0	3	0
4	В	299	0	0	4	0
4	С	330	0	0	6	0
4	D	288	0	0	3	0
4	aa	23	0	0	0	0
4	bb	27	0	0	0	0
4	сс	31	0	0	0	0
4	dd	25	0	0	0	0
All	All	13196	0	11930	100	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.

The worst 5 of 100 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:A:157:LEU:HB3	1:A:161:ILE:HD12	1.61	0.81
1:A:79:THR:HB	4:A:716:HOH:O	1.90	0.72



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASN:ND2	4:D:501:HOH:O	2.21	0.72
4:A:686[B]:HOH:O	1:D:248:ARG:NH2	2.26	0.68
1:C:318:LYS:HE2	4:C:520:HOH:O	1.97	0.65

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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	343/341~(101%)	335~(98%)	8 (2%)	0	100	100
1	В	343/341~(101%)	337~(98%)	6 (2%)	0	100	100
1	С	344/341~(101%)	339~(98%)	5 (2%)	0	100	100
1	D	343/341~(101%)	339~(99%)	4 (1%)	0	100	100
2	aa	30/35~(86%)	29~(97%)	1 (3%)	0	100	100
2	bb	31/35~(89%)	30~(97%)	1 (3%)	0	100	100
2	сс	32/35~(91%)	31 (97%)	1 (3%)	0	100	100
2	dd	30/35~(86%)	30 (100%)	0	0	100	100
All	All	1496/1504~(100%)	1470 (98%)	26 (2%)	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 side chain 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.



1 21 10
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	293/289~(101%)	292 (100%)	1 (0%)	92 95
1	В	293/289~(101%)	293 (100%)	0	100 100
1	С	294/289~(102%)	292~(99%)	2(1%)	84 88
1	D	293/289~(101%)	293 (100%)	0	100 100
2	aa	31/34~(91%)	31~(100%)	0	100 100
2	bb	32/34~(94%)	32~(100%)	0	100 100
2	cc	33/34~(97%)	33~(100%)	0	100 100
2	dd	31/34~(91%)	31~(100%)	0	100 100
All	All	1300/1292~(101%)	1297 (100%)	3(0%)	93 95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	264	GLU
1	С	107	SER
1	С	203	ARG

Sometimes 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 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,  $95^{th}$  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	$OWAB(A^2)$	Q < 0.9
1	А	341/341~(100%)	-0.22	4 (1%) 79 78	18, 27, 46, 73	0
1	В	341/341~(100%)	-0.24	3 (0%) 84 83	16, 25, 46, 79	0
1	С	341/341~(100%)	-0.35	1 (0%) 94 93	15, 23, 40, 70	0
1	D	341/341~(100%)	-0.22	3 (0%) 84 83	17, 27, 47, 69	0
2	aa	32/35~(91%)	-0.38	0 100 100	19, 24, 35, 51	0
2	bb	33/35~(94%)	-0.46	0 100 100	15, 21, 37, 51	0
2	сс	34/35~(97%)	-0.37	1 (2%) 51 50	16, 20, 42, 61	0
2	dd	32/35~(91%)	-0.58	0 100 100	18, 22, 30, 56	0
All	All	1495/1504~(99%)	-0.27	12 (0%) 86 85	15, 25, 45, 79	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	157	LEU	4.1
1	В	82	LEU	4.0
1	В	79	THR	2.8
1	D	1	LEU	2.8
1	D	112	VAL	2.7

### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	CL	С	401	1/1	0.97	0.07	36, 36, 36, 36	0
3	CL	D	401	1/1	0.97	0.06	41,41,41,41	0
3	CL	А	401	1/1	0.99	0.05	40,40,40,40	0
3	CL	В	401	1/1	0.99	0.04	38,38,38,38	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

