



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:32 AM UTC

PDB ID : 3SRJ / pdb\_00003srj  
Title : PfAMA1 in complex with invasion-inhibitory peptide R1  
Authors : Vulliez-Le Normand, B.; Saul, F.A.; Bentley, G.A.  
Deposited on : 2011-07-07  
Resolution : 2.15 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](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

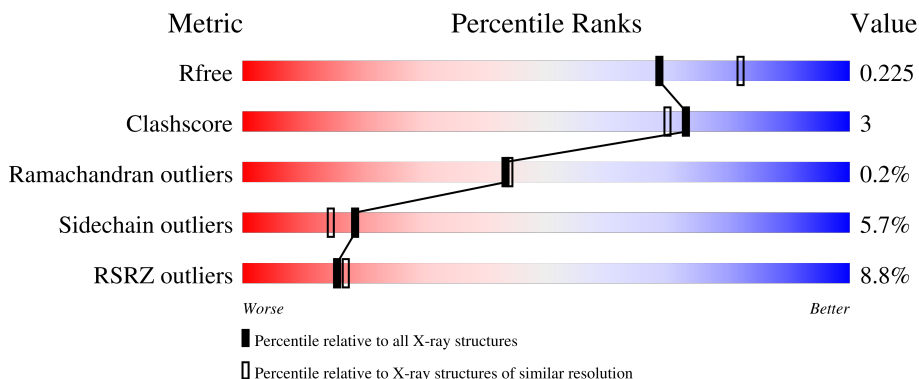
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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.



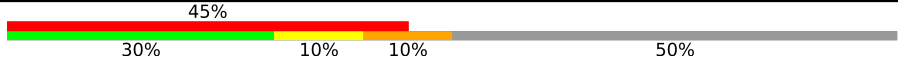
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	381	 3% 70% 7% 22%
1	B	381	 5% 71% 7% 22%
2	C	20	 15% 75% 15% 10%
2	D	20	 35% 15% 15% 5% 65%
2	E	20	 30% 80% 5% 15%

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Mol	Chain	Length	Quality of chain
2	F	20	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a green segment (30%), a yellow segment (10%), a red segment (10%), and a grey segment (50%). The total length of the bar is 100%. The green segment is labeled '30%', the yellow segment is labeled '10%', the red segment is labeled '10%', and the grey segment is labeled '50%'. Above the bar, the text '45%' is centered, indicating the combined percentage of the green and yellow segments.</p>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5639 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 Apical membrane antigen 1, AMA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2375	1505	398	455	17	0	0	0
1	B	297	2385	1515	398	454	18	0	3	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLU	-	expression tag	UNP Q7KQK5
A	96	PHE	-	expression tag	UNP Q7KQK5
A	162	LYS	ASN	engineered mutation	UNP Q7KQK5
A	288	VAL	THR	engineered mutation	UNP Q7KQK5
A	373	ASP	SER	engineered mutation	UNP Q7KQK5
A	422	ASP	ASN	engineered mutation	UNP Q7KQK5
A	423	LYS	SER	engineered mutation	UNP Q7KQK5
A	443	SER	-	expression tag	UNP Q7KQK5
A	444	VAL	-	expression tag	UNP Q7KQK5
A	445	PRO	-	expression tag	UNP Q7KQK5
A	446	ARG	-	expression tag	UNP Q7KQK5
A	447	ALA	-	expression tag	UNP Q7KQK5
A	448	ALA	-	expression tag	UNP Q7KQK5
A	449	ALA	-	expression tag	UNP Q7KQK5
A	450	ALA	-	expression tag	UNP Q7KQK5
A	451	ALA	-	expression tag	UNP Q7KQK5
A	452	SER	-	expression tag	UNP Q7KQK5
A	453	PHE	-	expression tag	UNP Q7KQK5
A	454	LEU	-	expression tag	UNP Q7KQK5
A	455	GLU	-	expression tag	UNP Q7KQK5
A	456	GLN	-	expression tag	UNP Q7KQK5
A	457	LYS	-	expression tag	UNP Q7KQK5
A	458	LEU	-	expression tag	UNP Q7KQK5
A	459	ILE	-	expression tag	UNP Q7KQK5
A	460	SER	-	expression tag	UNP Q7KQK5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	461	GLU	-	expression tag	UNP Q7KQK5
A	462	GLU	-	expression tag	UNP Q7KQK5
A	463	ASP	-	expression tag	UNP Q7KQK5
A	464	LEU	-	expression tag	UNP Q7KQK5
A	465	ASN	-	expression tag	UNP Q7KQK5
A	466	SER	-	expression tag	UNP Q7KQK5
A	467	ALA	-	expression tag	UNP Q7KQK5
A	468	VAL	-	expression tag	UNP Q7KQK5
A	469	ASP	-	expression tag	UNP Q7KQK5
A	470	HIS	-	expression tag	UNP Q7KQK5
A	471	HIS	-	expression tag	UNP Q7KQK5
A	472	HIS	-	expression tag	UNP Q7KQK5
A	473	HIS	-	expression tag	UNP Q7KQK5
A	474	HIS	-	expression tag	UNP Q7KQK5
A	475	HIS	-	expression tag	UNP Q7KQK5
B	95	GLU	-	expression tag	UNP Q7KQK5
B	96	PHE	-	expression tag	UNP Q7KQK5
B	162	LYS	ASN	engineered mutation	UNP Q7KQK5
B	288	VAL	THR	engineered mutation	UNP Q7KQK5
B	373	ASP	SER	engineered mutation	UNP Q7KQK5
B	422	ASP	ASN	engineered mutation	UNP Q7KQK5
B	423	LYS	SER	engineered mutation	UNP Q7KQK5
B	443	SER	-	expression tag	UNP Q7KQK5
B	444	VAL	-	expression tag	UNP Q7KQK5
B	445	PRO	-	expression tag	UNP Q7KQK5
B	446	ARG	-	expression tag	UNP Q7KQK5
B	447	ALA	-	expression tag	UNP Q7KQK5
B	448	ALA	-	expression tag	UNP Q7KQK5
B	449	ALA	-	expression tag	UNP Q7KQK5
B	450	ALA	-	expression tag	UNP Q7KQK5
B	451	ALA	-	expression tag	UNP Q7KQK5
B	452	SER	-	expression tag	UNP Q7KQK5
B	453	PHE	-	expression tag	UNP Q7KQK5
B	454	LEU	-	expression tag	UNP Q7KQK5
B	455	GLU	-	expression tag	UNP Q7KQK5
B	456	GLN	-	expression tag	UNP Q7KQK5
B	457	LYS	-	expression tag	UNP Q7KQK5
B	458	LEU	-	expression tag	UNP Q7KQK5
B	459	ILE	-	expression tag	UNP Q7KQK5
B	460	SER	-	expression tag	UNP Q7KQK5
B	461	GLU	-	expression tag	UNP Q7KQK5
B	462	GLU	-	expression tag	UNP Q7KQK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	463	ASP	-	expression tag	UNP Q7KQK5
B	464	LEU	-	expression tag	UNP Q7KQK5
B	465	ASN	-	expression tag	UNP Q7KQK5
B	466	SER	-	expression tag	UNP Q7KQK5
B	467	ALA	-	expression tag	UNP Q7KQK5
B	468	VAL	-	expression tag	UNP Q7KQK5
B	469	ASP	-	expression tag	UNP Q7KQK5
B	470	HIS	-	expression tag	UNP Q7KQK5
B	471	HIS	-	expression tag	UNP Q7KQK5
B	472	HIS	-	expression tag	UNP Q7KQK5
B	473	HIS	-	expression tag	UNP Q7KQK5
B	474	HIS	-	expression tag	UNP Q7KQK5
B	475	HIS	-	expression tag	UNP Q7KQK5

- Molecule 2 is a protein called R1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	S	0	1	0
			157	106	27	23	1			
2	D	7	Total	C	N	O		0	0	0
			60	43	7	10				
2	E	17	Total	C	N	O	S	0	0	0
			135	92	21	21	1			
2	F	10	Total	C	N	O		0	0	0
			77	54	10	13				

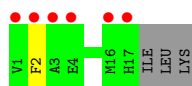
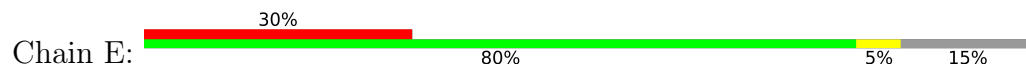
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total	O	0	0
			236	236		
3	B	196	Total	O	0	0
			196	196		
3	C	13	Total	O	0	0
			13	13		
3	D	1	Total	O	0	0
			1	1		
3	E	3	Total	O	0	0
			3	3		
3	F	1	Total	O	0	0
			1	1		

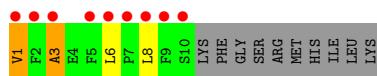
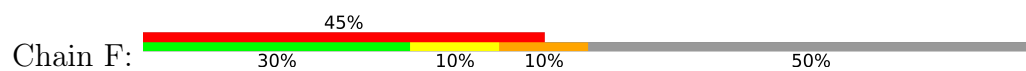




- Molecule 2: R1 peptide



- Molecule 2: R1 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.32Å 144.32Å 145.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.06 – 2.15 37.06 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (37.06-2.15) 94.7 (37.06-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.16Å)	Xtrriage
Refinement program	BUSTER 2.9.3	Depositor
R, $R_{free}$	0.171 , 0.214 0.178 , 0.225	Depositor DCC
$R_{free}$ test set	1297 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtrriage
Anisotropy	0.370	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.014 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.86	0/2437	1.23	7/3304 (0.2%)
1	B	0.84	0/2454	1.21	5/3327 (0.2%)
2	C	0.69	0/163	1.10	0/217
2	D	0.59	0/62	0.95	0/83
2	E	0.72	0/139	1.01	0/184
2	F	0.89	0/79	1.43	2/107 (1.9%)
All	All	0.84	0/5334	1.21	14/7222 (0.2%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	PHE	CA-CB-CG	7.03	120.83	113.80
1	A	444	VAL	CB-CA-C	6.34	117.25	110.53
1	A	439	ASN	N-CA-C	5.96	118.55	111.33
1	B	435	ILE	N-CA-C	5.94	116.31	111.62
2	F	3	ALA	CA-C-N	5.80	132.14	121.70

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	A	2375	0	2251	20	0
1	B	2385	0	2260	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	157	0	150	2	0
2	D	60	0	57	4	0
2	E	135	0	130	0	0
2	F	77	0	76	1	0
3	A	236	0	0	1	0
3	B	196	0	0	0	0
3	C	13	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
All	All	5639	0	4924	32	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 3.

The worst 5 of 32 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:297:ASN:HD22	1:B:297:ASN:H	1.33	0.74
1:A:233:ASN:HD22	1:A:233:ASN:H	1.37	0.70
1:A:297:ASN:HD22	1:A:297:ASN:H	1.38	0.70
1:A:136:GLU:H	1:A:233:ASN:HD21	1.43	0.66
1:B:335:PHE:HD1	1:B:434:PRO:HB2	1.62	0.63

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
1	A	292/381 (77%)	278 (95%)	13 (4%)	1 (0%)	36 34
1	B	294/381 (77%)	285 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	17/20 (85%)	14 (82%)	3 (18%)	0	100	100
2	D	5/20 (25%)	5 (100%)	0	0	100	100
2	E	15/20 (75%)	14 (93%)	1 (7%)	0	100	100
2	F	8/20 (40%)	5 (62%)	3 (38%)	0	100	100
All	All	631/842 (75%)	601 (95%)	29 (5%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ARG

### 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	A	262/336 (78%)	250 (95%)	12 (5%)	24	22
1	B	262/336 (78%)	250 (95%)	12 (5%)	24	22
2	C	16/18 (89%)	15 (94%)	1 (6%)	16	11
2	D	7/18 (39%)	4 (57%)	3 (43%)	0	0
2	E	13/18 (72%)	12 (92%)	1 (8%)	12	7
2	F	8/18 (44%)	5 (62%)	3 (38%)	0	0
All	All	568/744 (76%)	536 (94%)	32 (6%)	18	15

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	2	PHE
2	F	1	VAL
1	B	106	MET
1	A	444	VAL
2	F	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	309	ASN
1	B	297	ASN
1	A	421	ASN
1	A	319	ASN
1	A	439	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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 <sup>2</sup> )	Q<0.9
1	A	298/381 (78%)	-0.05	13 (4%) 39 44	20, 31, 67, 115	0
1	B	297/381 (77%)	0.15	19 (6%) 25 28	18, 35, 75, 100	3 (1%)
2	C	18/20 (90%)	0.82	3 (16%) 4 5	31, 43, 71, 83	1 (5%)
2	D	7/20 (35%)	3.72	7 (100%) 0 0	67, 73, 85, 99	0
2	E	17/20 (85%)	1.65	6 (35%) 1 1	43, 55, 85, 92	0
2	F	10/20 (50%)	4.16	9 (90%) 0 0	78, 87, 108, 109	0
All	All	647/842 (76%)	0.22	57 (8%) 15 17	18, 34, 81, 115	4 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	VAL	7.0
2	F	3	ALA	6.2
1	A	350	PRO	5.8
1	A	352	GLN	5.8
2	F	6	LEU	5.5

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.