



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:33 am GMT

PDB ID : 3SRJ
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

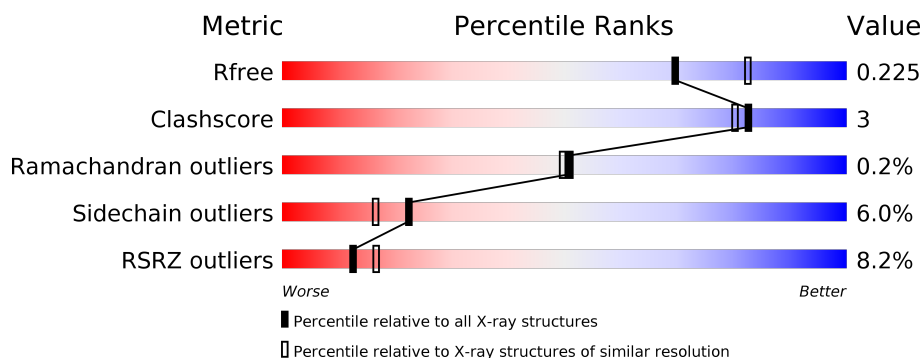
1 Overall quality at a glance

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}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>7%</div> <div>22%</div> </div> </div>
1	B	381	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>5%</div> <div>22%</div> </div> </div>
2	C	20	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>10%</div> </div> </div>
2	D	20	<div> <div>20%</div> <div> <div>20%</div> <div>10%</div> <div>5%</div> <div>65%</div> </div> </div>
2	E	20	<div> <div>35%</div> <div> <div></div> <div>80%</div> <div>5%</div> <div>15%</div> </div> </div>
2	F	20	<div> <div>35%</div> <div> <div>30%</div> <div>15%</div> <div>5%</div> <div>50%</div> </div> </div>

2 Entry composition

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
1	A	298	Total	C	N	O	S	0	0	0
			2375	1505	398	455	17			
1	B	297	Total	C	N	O	S	0	3	0
			2385	1515	398	454	18			

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

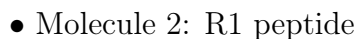
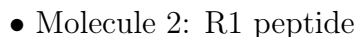
- Molecule 2 is a protein called R1 peptide.

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.

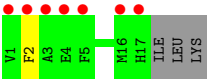
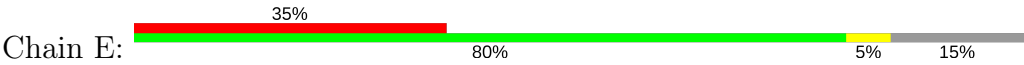
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total	O	0	0
			236	236		
3	B	196	Total	O	0	0
			196	196		
3	C	13	Total	O	0	0
			13	13		
3	D	1	Total	O	0	0
			1	1		
3	E	3	Total	O	0	0
			3	3		
3	F	1	Total	O	0	0
			1	1		

- Molecule 1: Apical membrane antigen 1, AMA1

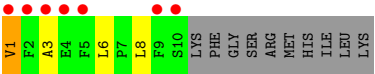
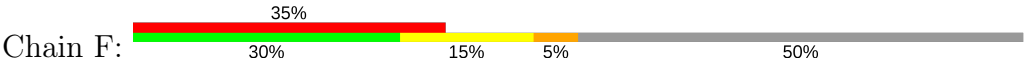




● Molecule 2: R1 peptide



● Molecule 2: R1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 94.8 (37.06-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.16Å)	Xtriage
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 (3.13%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5639	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.52	0/2437	0.68	0/3304
1	B	0.50	0/2454	0.67	0/3327
2	C	0.44	0/163	0.67	0/217
2	D	0.43	0/62	0.52	0/83
2	E	0.43	0/139	0.55	0/184
2	F	0.51	0/79	0.91	0/107
All	All	0.50	0/5334	0.67	0/7222

There are no bond length outliers.

There are no bond angle outliers.

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	19	0
1	B	2385	0	2260	8	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	0	0
3	F	1	0	0	0	0
All	All	5639	0	4924	29	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 29 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:H	1:B:297:ASN:HD22	1.33	0.74
1:A:233:ASN:H	1:A:233:ASN:HD22	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%)	44	41
1	B	294/381 (77%)	285 (97%)	9 (3%)	0	100	100
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%)	51	50

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%)	247 (94%)	15 (6%)	24	18
1	B	262/336 (78%)	250 (95%)	12 (5%)	31	27
2	C	16/18 (89%)	15 (94%)	1 (6%)	21	15
2	D	7/18 (39%)	5 (71%)	2 (29%)	0	0
2	E	13/18 (72%)	12 (92%)	1 (8%)	15	9
2	F	8/18 (44%)	5 (62%)	3 (38%)	0	0
All	All	568/744 (76%)	534 (94%)	34 (6%)	22	16

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	106	MET
1	B	195	LEU
2	F	1	VAL
1	B	178	ASP
1	A	258	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	B	297	ASN
1	B	223	ASN
1	A	210	ASN
1	B	286	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 carbohydrates 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, 95th 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	A	298/381 (78%)	0.05	16 (5%) 26 34	20, 31, 67, 115	0
1	B	297/381 (77%)	0.12	17 (5%) 24 32	18, 35, 76, 100	0
2	C	18/20 (90%)	0.63	2 (11%) 6 8	37, 46, 71, 83	0
2	D	7/20 (35%)	2.93	4 (57%) 0 0	67, 73, 85, 99	0
2	E	17/20 (85%)	1.89	7 (41%) 0 1	43, 55, 85, 92	0
2	F	10/20 (50%)	4.36	7 (70%) 0 0	78, 87, 108, 109	0
All	All	647/842 (76%)	0.25	53 (8%) 12 17	18, 35, 81, 115	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	VAL	8.4
1	A	260	PRO	8.4
2	E	1	VAL	8.3
1	A	445	PRO	8.1
1	A	106	MET	7.8

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.