



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:07 AM UTC

PDB ID : 5NQG / pdb_00005nqg
Title : Crystal structure of Plasmodium vivax AMA1 in complex with a 39 aa PvRON2 peptide
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Deposited on : 2017-04-20
Resolution : 2.15 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

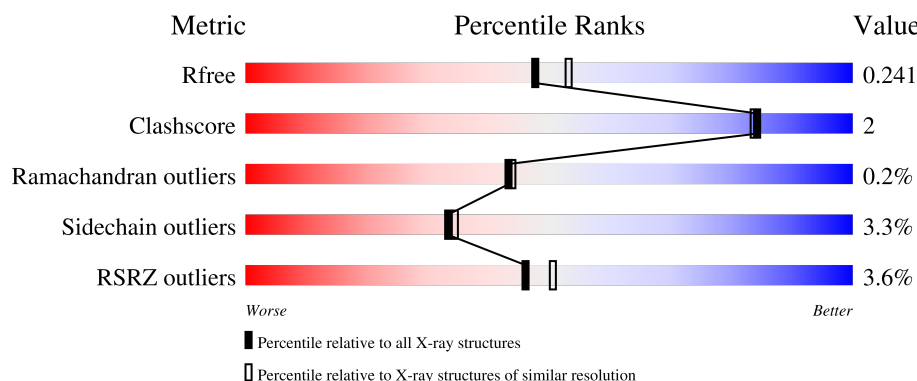
1 Overall quality at a glance

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 ≥ 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	471	 3% 73% 6% 19%
2	B	39	 79% 5% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3558 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 merozoite antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	3088	1938	538	586	26	0	3	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLU	-	expression tag	UNP O61130
A	40	ALA	-	expression tag	UNP O61130
A	41	SER	-	expression tag	UNP O61130
A	42	ILE	-	expression tag	UNP O61130
A	119	GLU	GLN	engineered mutation	UNP O61130
A	178	ASN	SER	engineered mutation	UNP O61130
A	226	ASP	ASN	engineered mutation	UNP O61130
A	441	GLN	ASN	engineered mutation	UNP O61130
A	488	LEU	-	expression tag	UNP O61130
A	489	GLU	-	expression tag	UNP O61130
A	490	GLN	-	expression tag	UNP O61130
A	491	LYS	-	expression tag	UNP O61130
A	492	LEU	-	expression tag	UNP O61130
A	493	ILE	-	expression tag	UNP O61130
A	494	SER	-	expression tag	UNP O61130
A	495	GLU	-	expression tag	UNP O61130
A	496	GLU	-	expression tag	UNP O61130
A	497	ASP	-	expression tag	UNP O61130
A	498	LEU	-	expression tag	UNP O61130
A	499	ASN	-	expression tag	UNP O61130
A	500	SER	-	expression tag	UNP O61130
A	501	ALA	-	expression tag	UNP O61130
A	502	VAL	-	expression tag	UNP O61130
A	503	ASP	-	expression tag	UNP O61130
A	504	HIS	-	expression tag	UNP O61130
A	505	HIS	-	expression tag	UNP O61130
A	506	HIS	-	expression tag	UNP O61130

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Chain	Residue	Modelled	Actual	Comment	Reference
A	507	HIS	-	expression tag	UNP O61130
A	508	HIS	-	expression tag	UNP O61130
A	509	HIS	-	expression tag	UNP O61130

- Molecule 2 is a protein called RON2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	33	Total	C	N	O	S	0	1	0
			236	145	40	48	3			

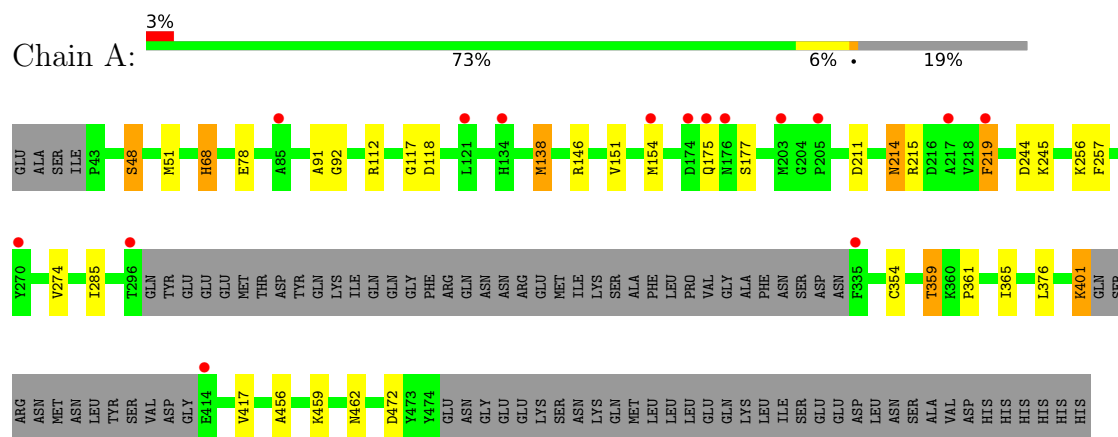
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	223	Total	O	0	0
			223	223		
3	B	11	Total	O	0	0
			11	11		

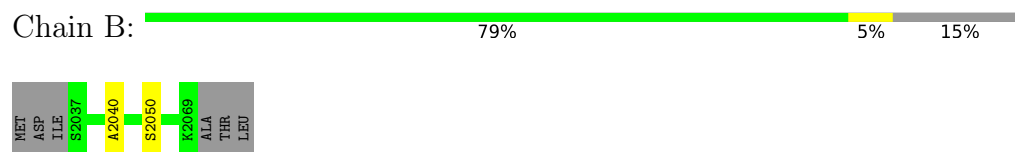
3 Residue-property plots [i](#)

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: Apical merozoite antigen 1



• Molecule 2: RON2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.46Å 54.00Å 62.13Å 90.00° 105.71° 90.00°	Depositor
Resolution (Å)	39.58 – 2.15 39.58 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (39.58-2.15) 97.6 (39.58-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.174 , 0.226 0.184 , 0.241	Depositor DCC
R_{free} test set	1641 reflections (5.82%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3558	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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

5.1 Standard geometry

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	0/3163	1.21	11/4260 (0.3%)
2	B	0.83	0/241	1.29	2/332 (0.6%)
All	All	0.86	0/3404	1.21	13/4592 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	PHE	CA-CB-CG	6.29	120.09	113.80
2	B	2040	ALA	CA-C-N	5.62	127.75	120.44
2	B	2040	ALA	C-N-CA	5.62	127.75	120.44
1	A	244	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	376	LEU	CA-C-N	5.45	128.97	120.75
1	A	376	LEU	C-N-CA	5.45	128.97	120.75
1	A	214	ASN	CA-C-N	5.39	129.31	120.63
1	A	214	ASN	C-N-CA	5.39	129.31	120.63
1	A	211	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	459	LYS	CA-C-N	5.23	128.01	120.38
1	A	459	LYS	C-N-CA	5.23	128.01	120.38
1	A	68	HIS	CA-C-N	5.05	129.72	122.40
1	A	68	HIS	C-N-CA	5.05	129.72	122.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3088	0	2986	15	0
2	B	236	0	216	0	0
3	A	223	0	0	0	0
3	B	11	0	0	0	0
All	All	3558	0	3202	15	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 (15) 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:274:VAL:HG21	1:A:285:ILE:HG21	1.72	0.71
1:A:274:VAL:HG23	1:A:354:CYS:HB3	1.78	0.64
1:A:78:GLU:HB2	1:A:91:ALA:HB2	1.84	0.59
1:A:175:GLN:C	1:A:177:SER:H	2.11	0.58
1:A:359:THR:HG21	1:A:462:ASN:HD22	1.69	0.57
1:A:68:HIS:CE1	1:A:92:GLY:HA3	2.42	0.55
1:A:256:LYS:HG2	1:A:365:ILE:HB	1.92	0.51
1:A:48:SER:HB2	1:A:417:VAL:HG12	1.96	0.48
1:A:51:MET:HE1	1:A:456:ALA:HB2	1.95	0.47
1:A:359:THR:HG21	1:A:462:ASN:ND2	2.30	0.47
1:A:401:LYS:HE3	1:A:417:VAL:H	1.82	0.45
1:A:359:THR:CG2	1:A:462:ASN:HD22	2.30	0.43
1:A:151:VAL:HA	1:A:154[A]:MET:HE3	2.01	0.42
1:A:138:MET:HE1	1:A:146:ARG:HD2	2.01	0.42
1:A:257:PHE:HB3	1:A:361:PRO:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	379/471 (80%)	367 (97%)	11 (3%)	1 (0%)	36	34
2	B	32/39 (82%)	31 (97%)	1 (3%)	0	100	100
All	All	411/510 (81%)	398 (97%)	12 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	GLY

5.3.2 Protein sidechains ⓘ

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	342/423 (81%)	331 (97%)	11 (3%)	34	36
2	B	26/33 (79%)	25 (96%)	1 (4%)	29	29
All	All	368/456 (81%)	356 (97%)	12 (3%)	33	34

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	112	ARG
1	A	118	ASP
1	A	138	MET
1	A	214	ASN
1	A	215	ARG
1	A	219	PHE
1	A	245	LYS
1	A	359	THR
1	A	401	LYS
1	A	472	ASP
2	B	2050	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	202	ASN
1	A	231	ASN
1	A	369	ASN
1	A	380	GLN
1	A	445	ASN
2	B	2066	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 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, 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	382/471 (81%)	0.14	15 (3%)	43 48	29, 43, 81, 114	3 (0%)
2	B	33/39 (84%)	0.83	0	100 100	30, 60, 84, 93	1 (3%)
All	All	415/510 (81%)	0.19	15 (3%)	46 50	29, 44, 83, 114	4 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203[A]	MET	4.0
1	A	175	GLN	4.0
1	A	176	ASN	3.0
1	A	296	THR	2.9
1	A	335	PHE	2.8
1	A	205	PRO	2.4
1	A	174	ASP	2.3
1	A	121	LEU	2.3
1	A	219	PHE	2.2
1	A	154[A]	MET	2.2
1	A	85	ALA	2.2
1	A	414	GLU	2.1
1	A	134[A]	HIS	2.1
1	A	270	TYR	2.0
1	A	217	ALA	2.0

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.