



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 08:14 PM EDT

PDB ID : 8GID  
Title : Crystal structure of a strain-transcending single-component Plasmodium falciparum AMA1-RON2L structure-based design immunogen 1 (SBD1)  
Authors : Patel, P.N.; Tolia, N.H.  
Deposited on : 2023-03-14  
Resolution : 1.80 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

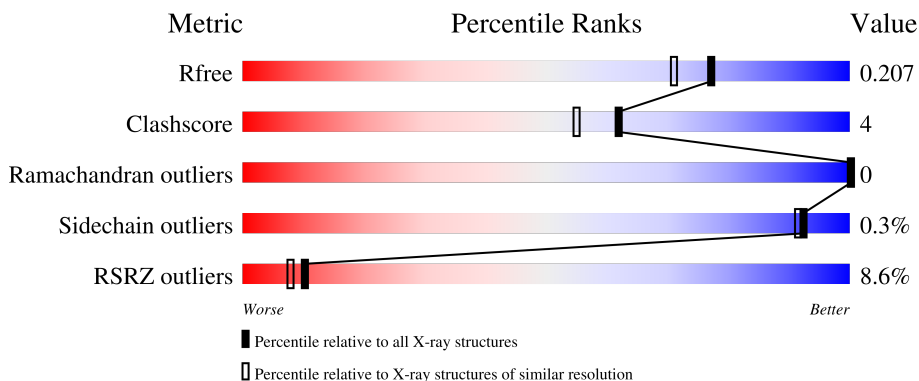
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	377	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5425 atoms, of which 2569 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, rhoptry neck protein 2 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	339	5261	1696	2569	458	519	19	0	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	expression tag	UNP D9MXR5
A	-1	THR	-	expression tag	UNP D9MXR5
A	0	GLY	-	expression tag	UNP D9MXR5
A	38	ALA	SER	engineered mutation	UNP D9MXR5
A	39	ALA	SER	engineered mutation	UNP D9MXR5
A	54	GLY	-	linker	UNP D9MXR5
A	55	GLY	-	linker	UNP D9MXR5
A	56	GLY	-	linker	UNP D9MXR5
A	57	GLY	-	linker	UNP D9MXR5
A	58	SER	-	linker	UNP D9MXR5
A	59	GLY	-	linker	UNP D9MXR5
A	60	GLY	-	linker	UNP D9MXR5
A	61	GLY	-	linker	UNP D9MXR5
A	62	GLY	-	linker	UNP D9MXR5
A	63	SER	-	linker	UNP D9MXR5
A	64	GLY	-	linker	UNP D9MXR5
A	65	GLY	-	linker	UNP D9MXR5
A	66	GLY	-	linker	UNP D9MXR5
A	67	GLY	-	linker	UNP D9MXR5
A	68	SER	-	linker	UNP D9MXR5
A	69	GLY	-	linker	UNP D9MXR5
A	70	GLY	-	linker	UNP D9MXR5
A	71	GLY	-	linker	UNP D9MXR5
A	72	GLY	-	linker	UNP D9MXR5
A	134	ALA	THR	engineered mutation	UNP Q7KQK5
A	258	ALA	THR	engineered mutation	UNP Q7KQK5
A	366	GLY	-	expression tag	UNP Q8IKV6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	367	THR	-	expression tag	UNP Q8IKV6
A	368	LYS	-	expression tag	UNP Q8IKV6
A	369	HIS	-	expression tag	UNP Q8IKV6
A	370	HIS	-	expression tag	UNP Q8IKV6
A	371	HIS	-	expression tag	UNP Q8IKV6
A	372	HIS	-	expression tag	UNP Q8IKV6
A	373	HIS	-	expression tag	UNP Q8IKV6
A	374	HIS	-	expression tag	UNP Q8IKV6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	164	Total O 164 164	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.62Å 38.34Å 71.97Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	19.81 – 1.80 19.81 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.81-1.80) 97.1 (19.81-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.178 , 0.209 0.177 , 0.207	Depositor DCC
$R_{free}$ test set	1638 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% 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	0.35	0/2759	0.57	0/3742

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	2692	2569	2568	23	0
2	A	164	0	0	3	0
All	All	2856	2569	2568	23	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 4.

All (23) 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:278:GLN:NE2	2:A:401:HOH:O	2.26	0.68
1:A:98:ARG:NH1	2:A:402:HOH:O	2.30	0.64
1:A:360:VAL:CG1	1:A:364:LEU:HD12	2.27	0.64
1:A:114:LEU:HD21	1:A:204:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HD11	1:A:347:ARG:CG	2.35	0.57
1:A:154:PRO:HG2	1:A:356:LEU:HD22	1.87	0.56
1:A:104:ASP:HB3	1:A:111:GLN:HG2	1.88	0.55
1:A:195:ILE:HD11	1:A:347:ARG:HG2	1.88	0.55
1:A:226:GLU:OE2	1:A:228:ASN:ND2	2.40	0.54
1:A:51:GLU:OE2	1:A:274:ARG:NH2	2.38	0.51
1:A:360:VAL:HG11	1:A:364:LEU:HD12	1.95	0.48
1:A:156:THR:HG22	1:A:356:LEU:HD23	1.93	0.48
1:A:182:ASP:OD1	1:A:183:GLU:N	2.48	0.47
1:A:114:LEU:HD21	1:A:204:TYR:CE2	2.50	0.46
1:A:179:LYS:NZ	2:A:410:HOH:O	2.49	0.45
1:A:139:VAL:CG2	1:A:364:LEU:HD11	2.48	0.44
1:A:139:VAL:HG12	1:A:154:PRO:HD3	1.98	0.44
1:A:192:GLY:O	1:A:347:ARG:HD2	2.19	0.41
1:A:195:ILE:HD11	1:A:347:ARG:HG3	2.02	0.41
1:A:51:GLU:OE1	1:A:274:ARG:NH1	2.43	0.41
1:A:182:ASP:OD2	1:A:269:GLU:OE2	2.39	0.41
1:A:147:LYS:NZ	1:A:236:ASP:O	2.52	0.40
1:A:172:TYR:HB3	1:A:178:VAL:HG23	2.04	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
1	A	335/377 (89%)	327 (98%)	8 (2%)	0	<a href="#">100</a> <a href="#">100</a>

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	296/315 (94%)	295 (100%)	1 (0%)	<a href="#">92</a> <a href="#">91</a>

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	PHE

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](#)

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	339/377 (89%)	0.36	29 (8%) <b>10</b> <b>8</b>	19, 32, 63, 80	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	THR	6.4
1	A	77	GLY	6.2
1	A	340	VAL	5.4
1	A	4	ARG	5.0
1	A	236	ASP	4.3
1	A	230	PRO	4.1
1	A	235	LYS	4.0
1	A	143	ASN	3.9
1	A	323	TYR	3.7
1	A	231	ARG	3.6
1	A	362	THR	3.3
1	A	3	ASP	3.1
1	A	282	PHE	3.0
1	A	349	SER	2.9
1	A	200	LYS	2.9
1	A	328	THR	2.7
1	A	239	LYS	2.7
1	A	351	PRO	2.5
1	A	198	ASN	2.5
1	A	228	ASN	2.4
1	A	350	PRO	2.4
1	A	142	GLY	2.3
1	A	327	LEU	2.3
1	A	232	TYR	2.2
1	A	287	ASP	2.2
1	A	145	TYR	2.1
1	A	330	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	2.0
1	A	289	ASN	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 monosaccharides 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.