Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 08:20 PM EDT

PDB ID	:	8GIE
Title	:	Crystal structure of a designed single-component Plasmodium falciparum AMA1-RON2L insertion fusion immunogen 2
Authors	:	Patel, P.N.; Tolia, N.H.
Deposited on	:	2023-03-14
Resolution	:	1.85 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:

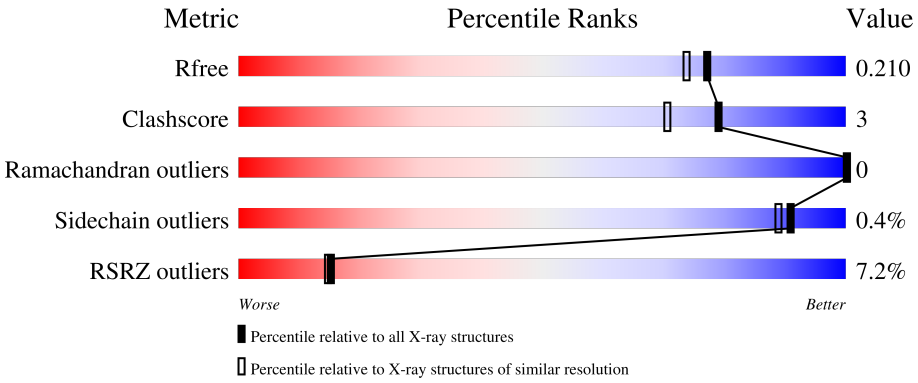
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	A	349	6% 82% 6% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4813 atoms, of which 2297 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	305	4704	1525	2297	402	462	18	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP Q7KQK5
A	2	THR	-	expression tag	UNP Q7KQK5
A	3	GLY	-	expression tag	UNP Q7KQK5
A	64	ALA	THR	engineered mutation	UNP Q7KQK5
A	160	GLY	-	linker	UNP Q7KQK5
A	161	GLY	-	linker	UNP Q7KQK5
A	162	GLY	-	linker	UNP Q7KQK5
A	163	GLY	-	linker	UNP Q7KQK5
A	164	SER	-	linker	UNP Q7KQK5
A	165	GLY	-	linker	UNP Q7KQK5
A	166	SER	-	linker	UNP Q7KQK5
A	206	GLY	-	linker	UNP Q8IKV6
A	207	GLY	-	linker	UNP Q8IKV6
A	208	SER	-	linker	UNP Q8IKV6
A	209	GLY	-	linker	UNP Q8IKV6
A	225	ALA	THR	engineered mutation	UNP Q7KQK5
A	?	-	LYS	deletion	UNP Q7KQK5
A	?	-	GLN	deletion	UNP Q7KQK5
A	?	-	TYR	deletion	UNP Q7KQK5
A	?	-	GLU	deletion	UNP Q7KQK5
A	?	-	GLN	deletion	UNP Q7KQK5
A	?	-	HIS	deletion	UNP Q7KQK5
A	?	-	LEU	deletion	UNP Q7KQK5
A	?	-	THR	deletion	UNP Q7KQK5
A	?	-	ASP	deletion	UNP Q7KQK5
A	?	-	TYR	deletion	UNP Q7KQK5
A	?	-	GLU	deletion	UNP Q7KQK5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q7KQK5
A	?	-	ILE	deletion	UNP Q7KQK5
A	?	-	LYS	deletion	UNP Q7KQK5
A	?	-	GLU	deletion	UNP Q7KQK5
A	?	-	GLY	deletion	UNP Q7KQK5
A	?	-	PHE	deletion	UNP Q7KQK5
A	?	-	LYS	deletion	UNP Q7KQK5
A	?	-	ASN	deletion	UNP Q7KQK5
A	?	-	LYS	deletion	UNP Q7KQK5
A	?	-	ASN	deletion	UNP Q7KQK5
A	?	-	ALA	deletion	UNP Q7KQK5
A	?	-	SER	deletion	UNP Q7KQK5
A	?	-	MET	deletion	UNP Q7KQK5
A	?	-	ILE	deletion	UNP Q7KQK5
A	?	-	LYS	deletion	UNP Q7KQK5
A	?	-	SER	deletion	UNP Q7KQK5
A	?	-	ALA	deletion	UNP Q7KQK5
A	?	-	PHE	deletion	UNP Q7KQK5
A	?	-	LEU	deletion	UNP Q7KQK5
A	?	-	PRO	deletion	UNP Q7KQK5
A	?	-	THR	deletion	UNP Q7KQK5
A	?	-	GLY	deletion	UNP Q7KQK5
A	?	-	ALA	deletion	UNP Q7KQK5
A	?	-	PHE	deletion	UNP Q7KQK5
A	288	GLY	LYS	conflict	UNP Q7KQK5
A	289	GLY	ALA	conflict	UNP Q7KQK5
A	290	SER	ASP	conflict	UNP Q7KQK5
A	291	GLY	ARG	conflict	UNP Q7KQK5
A	325	ALA	SER	engineered mutation	UNP Q7KQK5
A	326	ALA	SER	engineered mutation	UNP Q7KQK5
A	341	GLY	-	expression tag	UNP Q7KQK5
A	342	THR	-	expression tag	UNP Q7KQK5
A	343	LYS	-	expression tag	UNP Q7KQK5
A	344	HIS	-	expression tag	UNP Q7KQK5
A	345	HIS	-	expression tag	UNP Q7KQK5
A	346	HIS	-	expression tag	UNP Q7KQK5
A	347	HIS	-	expression tag	UNP Q7KQK5
A	348	HIS	-	expression tag	UNP Q7KQK5
A	349	HIS	-	expression tag	UNP Q7KQK5

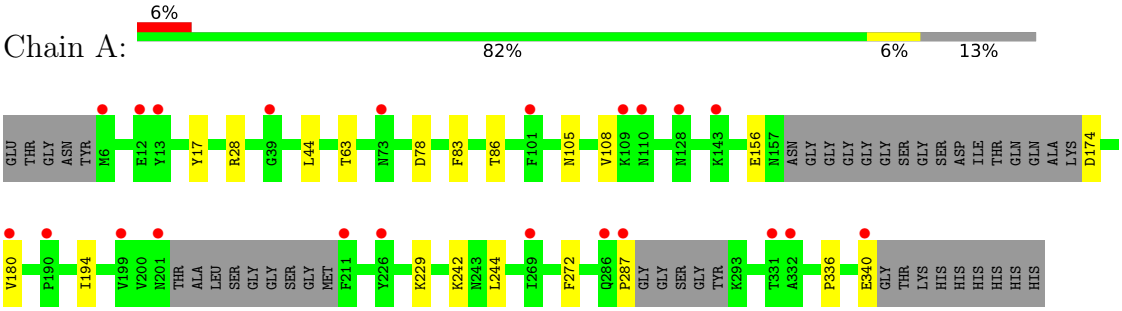
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	109	Total O 109 109	0	0

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 membrane antigen 1, rhoptry neck protein 2 chimera



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.63Å 62.83Å 60.47Å 90.00° 96.47° 90.00°	Depositor
Resolution (Å)	19.22 – 1.85 19.22 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.22-1.85) 97.7 (19.22-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.212 0.189 , 0.210	Depositor DCC
R_{free} test set	1269 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4813	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.29	0/2467	0.50	0/3347

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

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	2407	2297	2295	13	0
2	A	109	0	0	0	0
All	All	2516	2297	2295	13	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.

All (13) 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:17:TYR:OH	1:A:244:LEU:HD11	2.09	0.53
1:A:28:ARG:NH2	1:A:156:GLU:OE1	2.42	0.53
1:A:63:THR:OG1	1:A:78:ASP:OD2	2.30	0.48
1:A:174:ASP:O	1:A:287:PRO:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:O	1:A:108:VAL:HG22	2.16	0.45
1:A:174:ASP:N	1:A:174:ASP:OD1	2.49	0.44
1:A:44:LEU:HD12	1:A:44:LEU:C	2.38	0.44
1:A:180:VAL:HG12	1:A:180:VAL:O	2.18	0.43
1:A:242:LYS:HB2	1:A:340:GLU:HG3	2.01	0.43
1:A:242:LYS:HB2	1:A:340:GLU:CG	2.51	0.41
1:A:86:THR:HB	1:A:194:ILE:CG2	2.50	0.41
1:A:44:LEU:HD11	1:A:229:LYS:CE	2.51	0.41
1:A:272:PHE:CD1	1:A:336:PRO:HB2	2.56	0.41

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	297/349 (85%)	289 (97%)	8 (3%)	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 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	265/293 (90%)	264 (100%)	1 (0%)	91 89

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

Mol	Chain	Res	Type
1	A	83	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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^{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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	305/349 (87%)	0.49	22 (7%)	15	15	19, 32, 55, 75	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	MET	6.2
1	A	287	PRO	5.4
1	A	180	VAL	4.8
1	A	128	ASN	4.6
1	A	201	ASN	4.5
1	A	211	PHE	3.9
1	A	269	ILE	3.8
1	A	199	VAL	3.6
1	A	143	LYS	3.1
1	A	73	ASN	3.0
1	A	13	TYR	2.9
1	A	12	GLU	2.9
1	A	190	PRO	2.7
1	A	332	ALA	2.7
1	A	110	ASN	2.6
1	A	101	PHE	2.5
1	A	331	THR	2.4
1	A	109	LYS	2.4
1	A	286	GLN	2.3
1	A	226	TYR	2.1
1	A	39	GLY	2.1
1	A	340	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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.