



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:59 PM UTC

PDB ID : 8REK / pdb_00008rek
Title : Plasmodium vivax Apical Membrane Antigen 1/Fab complex
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Deposited on : 2023-12-11
Resolution : 3.05 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

<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
Mogul : 2022.3.0, CSD as543be (2022)
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

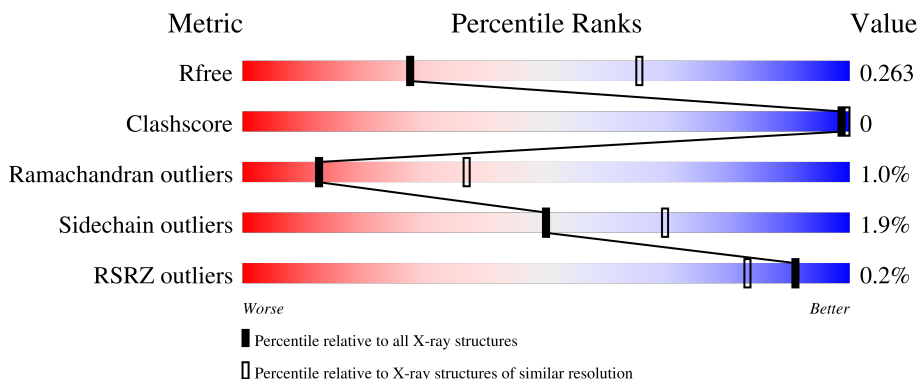
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	469	 75% 9% 15%
2	H	220	 89% 6% 5%
3	L	213	 92% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6293 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 (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3140	1968	539	609	24			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	-	expression tag	UNP Q9TY14
A	42	ILE	-	expression tag	UNP Q9TY14
A	178	ASN	SER	engineered mutation	UNP Q9TY14
A	226	ASP	ASN	engineered mutation	UNP Q9TY14
A	441	GLN	ASN	engineered mutation	UNP Q9TY14
A	488	LEU	-	expression tag	UNP Q9TY14
A	489	GLU	-	expression tag	UNP Q9TY14
A	490	GLN	-	expression tag	UNP Q9TY14
A	491	LYS	-	expression tag	UNP Q9TY14
A	492	LEU	-	expression tag	UNP Q9TY14
A	493	ILE	-	expression tag	UNP Q9TY14
A	494	SER	-	expression tag	UNP Q9TY14
A	495	GLU	-	expression tag	UNP Q9TY14
A	496	GLU	-	expression tag	UNP Q9TY14
A	497	ASP	-	expression tag	UNP Q9TY14
A	498	LEU	-	expression tag	UNP Q9TY14
A	499	ASN	-	expression tag	UNP Q9TY14
A	500	SER	-	expression tag	UNP Q9TY14
A	501	ALA	-	expression tag	UNP Q9TY14
A	502	VAL	-	expression tag	UNP Q9TY14
A	503	ASP	-	expression tag	UNP Q9TY14
A	504	HIS	-	expression tag	UNP Q9TY14
A	505	HIS	-	expression tag	UNP Q9TY14
A	506	HIS	-	expression tag	UNP Q9TY14
A	507	HIS	-	expression tag	UNP Q9TY14
A	508	HIS	-	expression tag	UNP Q9TY14
A	509	HIS	-	expression tag	UNP Q9TY14

- Molecule 2 is a protein called Fab 8.1.1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	0	0	0
			1558	988	252	310	8			

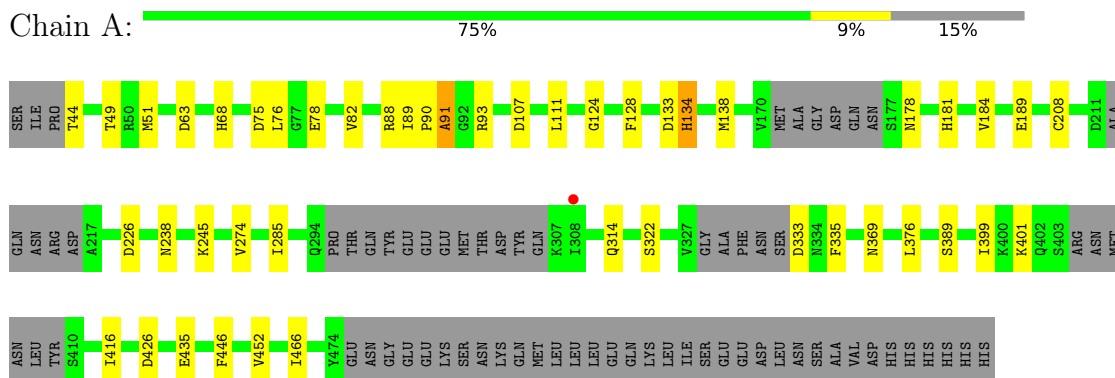
- Molecule 3 is a protein called Fab 8.1.1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1595	995	265	328	7			

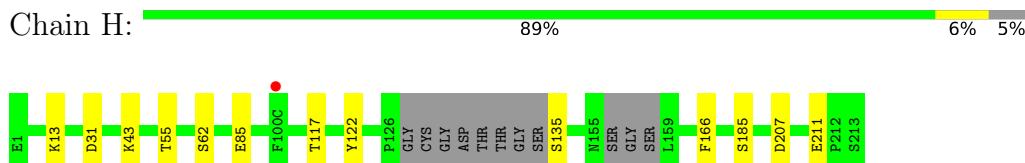
3 Residue-property plots

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.

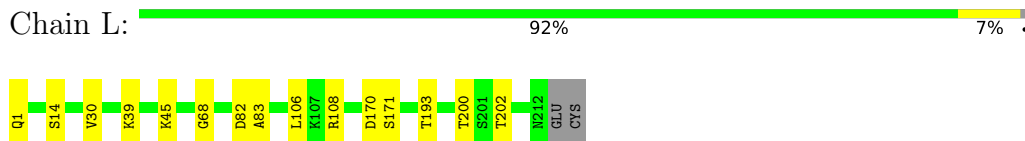
- Molecule 1: Apical membrane antigen 1 (Fragment)



- Molecule 2: Fab 8.1.1 heavy chain



- Molecule 3: Fab 8.1.1 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.39Å 214.68Å 57.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.54 – 3.05 69.54 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (69.54-3.05) 99.9 (69.54-3.05)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.221 , 0.292 (Not available) , 0.263	Depositor DCC
R_{free} test set	946 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	81.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6293	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	1.60	25/3202 (0.8%)	1.30	7/4321 (0.2%)
2	H	1.46	7/1598 (0.4%)	1.13	0/2184
3	L	1.50	5/1630 (0.3%)	1.14	1/2229 (0.0%)
All	All	1.54	37/6430 (0.6%)	1.22	8/8734 (0.1%)

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	HIS	CG-CD2	-11.04	1.23	1.35
1	A	134	HIS	C-N	7.87	1.43	1.33
2	H	13	LYS	C-N	7.41	1.41	1.33
1	A	389	SER	C-N	7.03	1.43	1.33
1	A	89	ILE	C-N	6.96	1.41	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	PHE	CA-CB-CG	6.48	120.28	113.80
1	A	226	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	426	ASP	CA-CB-CG	6.12	118.72	112.60
3	L	170	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	63	ASP	CA-CB-CG	5.40	118.00	112.60

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	3140	0	2962	5	0
2	H	1558	0	1478	1	0
3	L	1595	0	1482	0	0
All	All	6293	0	5922	6	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 0.

The worst 5 of 6 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)
2:H:135:SER:N	2:H:185:SER:HG	2.07	0.52
1:A:274:VAL:HG21	1:A:285:ILE:HG21	1.94	0.48
1:A:82:VAL:HG11	1:A:322:SER:HB3	1.97	0.46
1:A:51:MET:HE1	1:A:466:ILE:HD12	1.98	0.45
1:A:111:LEU:HD21	1:A:184:VAL:HG11	2.01	0.42

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	385/469 (82%)	347 (90%)	35 (9%)	3 (1%)	16 42
2	H	203/220 (92%)	190 (94%)	12 (6%)	1 (0%)	24 52
3	L	209/213 (98%)	188 (90%)	17 (8%)	4 (2%)	6 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	797/902 (88%)	725 (91%)	64 (8%)	8 (1%)	12 37

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	171	SER
3	L	202	THR
1	A	133	ASP
3	L	68	GLY
3	L	83	ALA

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	342/421 (81%)	336 (98%)	6 (2%)	51 70
2	H	171/186 (92%)	168 (98%)	3 (2%)	51 70
3	L	177/185 (96%)	173 (98%)	4 (2%)	44 66
All	All	690/792 (87%)	677 (98%)	13 (2%)	50 69

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	207	ASP
2	H	211	GLU
3	L	200	THR
3	L	106	LEU
3	L	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	334	ASN

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Mol	Chain	Res	Type
3	L	161	ASN
3	L	190	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PCA	L	1	3	7,8,9	1.36	1 (14%)	9,10,12	0.95	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	L	1	3	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1	PCA	O-C	3.05	1.31	1.20

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	PCA	O-C-CA	-2.77	117.65	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	397/469 (84%)	-0.33	1 (0%) 90 80	45, 82, 154, 176	0
2	H	209/220 (95%)	-0.15	1 (0%) 87 72	68, 113, 160, 180	0
3	L	210/213 (98%)	-0.45	0 100 100	62, 106, 138, 155	0
All	All	816/902 (90%)	-0.32	2 (0%) 91 83	45, 97, 151, 180	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	100(C)	PHE	3.0
1	A	308	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PCA	L	1	8/9	0.88	0.08	93,106,113,118	0

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.