WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:52 AM GMT

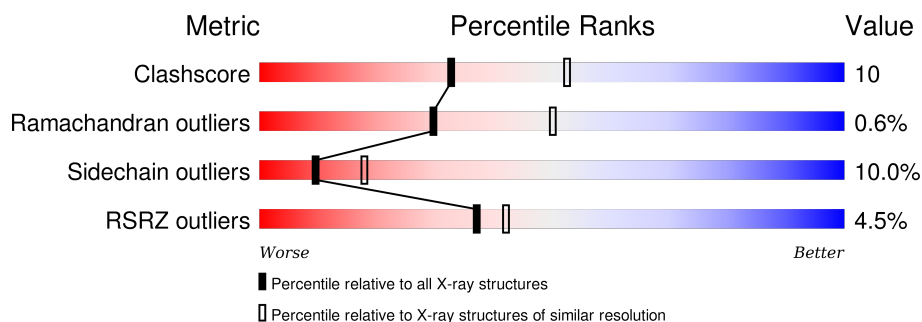|		
PDB ID	:	2J4W
Title	:	STRUCTURE OF A PLASMODIUM VIVAX APICAL MEMBRANE ANTI-GEN 1-FAB F8.12.19 COMPLEX
Authors	:	Igonet, S.; Vulliez-Le Normand, B.; Faure, G.; Riottot, M.M.; Kocken, C.H.M.; Thomas, A.W.; Bentley, G.A.
Deposited on	:	2006-09-07
Resolution	:	2.50 Å(reported)

---

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 2.50 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0.6%
Sidechain outliers		10.0%
RSRZ outliers		4.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	D	445	2% / 5% · 92%
2	H	225	4% / 76% 18% 5%
3	L	213	2% / 77% 19% · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3773 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	34	Total 270	C 167	N 43	O 55	S 5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	178	ASN	SER	ENGINEERED MUTATION	UNP Q9TY14
D	226	ASP	ASN	ENGINEERED MUTATION	UNP Q9TY14
D	441	GLU	ASN	ENGINEERED MUTATION	UNP Q9TY14

- Molecule 2 is a protein called FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total 1701	C 1075	N 278	O 340	S 8	0	0	0

- Molecule 3 is a protein called FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total 1647	C 1019	N 286	O 334	S 8	0	2	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total 4	O 4	0	0
4	H	61	Total 61	O 61	0	0
4	L	90	Total 90	O 90	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain D:

• Molecule 2: FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19

Chain H:

• Molecule 3: FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19

Chain L:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	171.79Å 171.79Å 44.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.50) 98.7 (19.84-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.187 , 0.241 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.5	EDS
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 26193 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3773	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	D	0.82	0/274	0.73	0/368
2	H	0.85	1/1745 (0.1%)	0.93	6/2381 (0.3%)
3	L	5.28	4/1691 (0.2%)	2.07	11/2298 (0.5%)
All	All	3.62	5/3710 (0.1%)	1.55	17/5047 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	49[A]	HIS	CD2-NE2	131.22	4.26	1.38
3	L	49[B]	HIS	CD2-NE2	131.22	4.26	1.38
3	L	49[A]	HIS	CG-CD2	76.12	2.65	1.35
3	L	49[B]	HIS	CG-CD2	76.12	2.65	1.35
2	H	208	CYS	CB-SG	-8.39	1.68	1.82

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	49[A]	HIS	CG-CD2-NE2	-44.05	25.50	109.20
3	L	49[B]	HIS	CG-CD2-NE2	-44.05	25.50	109.20
3	L	49[A]	HIS	ND1-CG-CD2	-33.39	59.25	106.00
3	L	49[B]	HIS	ND1-CG-CD2	-33.39	59.25	106.00
3	L	49[A]	HIS	CE1-NE2-CD2	-24.26	45.95	106.60

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	D	270	0	254	9	0
2	H	1701	0	1649	36	0
3	L	1647	0	1566	36	0
4	D	4	0	0	0	0
4	H	61	0	0	0	0
4	L	90	0	0	2	0
All	All	3773	0	3469	74	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 10.

The worst 5 of 74 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)
3:L:49[B]:HIS:CD2	3:L:49[B]:HIS:HB2	1.58	1.37
3:L:49[A]:HIS:CD2	3:L:49[A]:HIS:HB3	1.71	1.25
3:L:49[A]:HIS:CD2	3:L:49[A]:HIS:ND1	2.28	1.02
3:L:49[B]:HIS:CD2	3:L:49[B]:HIS:CB	2.44	1.01
3:L:49[A]:HIS:CD2	3:L:49[A]:HIS:CB	2.48	0.97

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	D	32/445 (7%)	28 (88%)	4 (12%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	223/225 (99%)	209 (94%)	13 (6%)	1 (0%)	39	61
3	L	213/213 (100%)	201 (94%)	10 (5%)	2 (1%)	21	37
All	All	468/883 (53%)	438 (94%)	27 (6%)	3 (1%)	30	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	128	SER
3	L	153	SER
3	L	151	ASP

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	D	34/397 (9%)	32 (94%)	2 (6%)	24	44
2	H	192/192 (100%)	170 (88%)	22 (12%)	7	13
3	L	188/186 (101%)	171 (91%)	17 (9%)	12	22
All	All	414/775 (53%)	373 (90%)	41 (10%)	9	18

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	198	PRO
2	H	218	LYS
3	L	207	LYS
2	H	199	ARG
2	H	204	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	124	GLN
3	L	190	ASN
2	H	135	ASN
3	L	161	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	1.59	1 (14%)	9,10,12	3.71	5 (55%)

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	CD-N	4.00	1.47	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1	PCA	CA-N-CD	-9.28	82.71	113.81
3	L	1	PCA	CB-CG-CD	-3.25	97.62	104.22
3	L	1	PCA	O-C-CA	-2.72	118.26	125.44
3	L	1	PCA	CB-CA-N	2.05	109.20	103.20
3	L	1	PCA	CB-CA-C	2.91	116.74	112.76

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 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(Å²)	Q<0.9
1	D	34/445 (7%)	1.09	8 (23%)	1	1	37, 57, 91, 94	0
2	H	225/225 (100%)	-0.18	9 (4%)	42	47	25, 38, 67, 99	0
3	L	212/213 (99%)	-0.33	4 (1%)	70	73	23, 36, 61, 100	1 (0%)
All	All	471/883 (53%)	-0.16	21 (4%)	37	42	23, 38, 72, 100	1 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	233	CYS	10.7
3	L	214	CYS	9.0
1	D	443	THR	8.2
2	H	130	ALA	7.5
1	D	422	PHE	7.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
3	PCA	L	1	8/9	0.91	0.21	-	57,59,61,61	0

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.