



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 11:36 AM EDT

PDB ID : 8DFH  
Title : Crystal structure of non-neutralizing / interfering human monoclonal antibody  
42C3 Fab in complex with MSP1-19  
Authors : Patel, P.N.; Tang, W.K.; Tolia, N.H.  
Deposited on : 2022-06-22  
Resolution : 2.30 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](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 : 2.35.1  
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

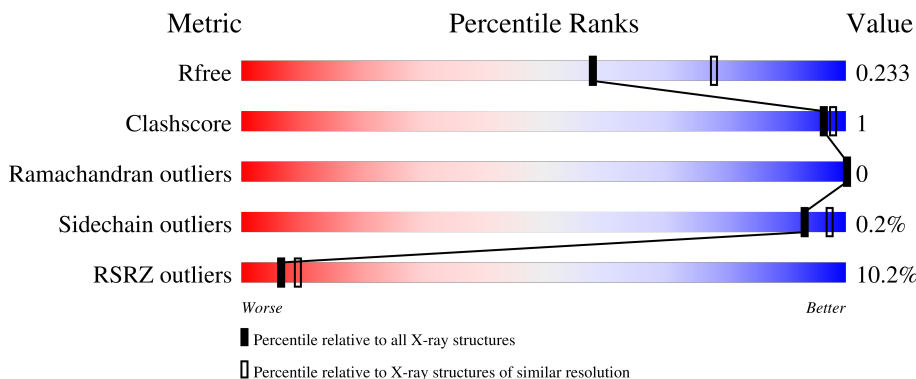
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	105	
2	H	238	
3	L	216	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7739 atoms, of which 3745 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 Merozoite surface protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	92	1348	423	638	125	150	12	0	2	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	expression tag	UNP Q8I0U8
A	-1	THR	-	expression tag	UNP Q8I0U8
A	0	GLY	-	expression tag	UNP Q8I0U8
A	3	ALA	SER	engineered mutation	UNP Q8I0U8
A	48	ALA	THR	engineered mutation	UNP Q8I0U8
A	94	GLY	-	expression tag	UNP Q8I0U8
A	95	THR	-	expression tag	UNP Q8I0U8
A	96	LYS	-	expression tag	UNP Q8I0U8
A	97	HIS	-	expression tag	UNP Q8I0U8
A	98	HIS	-	expression tag	UNP Q8I0U8
A	99	HIS	-	expression tag	UNP Q8I0U8
A	100	HIS	-	expression tag	UNP Q8I0U8
A	101	HIS	-	expression tag	UNP Q8I0U8
A	102	HIS	-	expression tag	UNP Q8I0U8

- Molecule 2 is a protein called 42C3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	H	218	3215	1041	1565	282	321	6	0	1	0

- Molecule 3 is a protein called 42C3 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	L	211	3125	990	1542	273	316	4	0	0	0

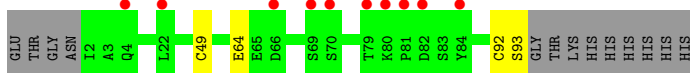
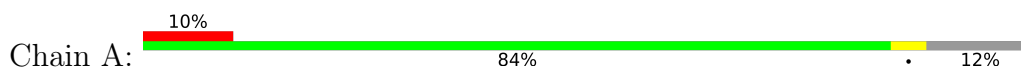
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	17	Total 17	O 17	0	0
4	H	17	Total 17	O 17	0	0
4	L	17	Total 17	O 17	0	0

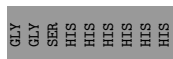
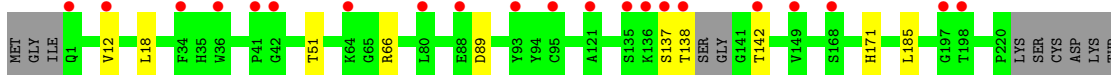
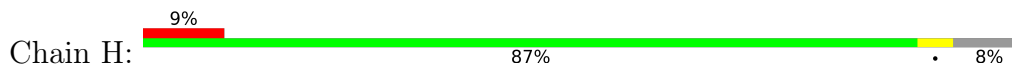
### 3 Residue-property plots [i](#)

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.

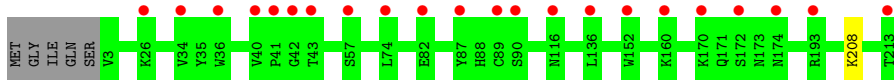
- Molecule 1: Merozoite surface protein 1



- Molecule 2: 42C3 Fab Heavy Chain



- Molecule 3: 42C3 Fab Light Chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.39Å 75.72Å 117.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.30 19.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.83-2.30) 96.7 (19.83-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.30Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.209 , 0.233 0.209 , 0.233	Depositor DCC
$R_{free}$ test set	1424 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.010 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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	0.26	0/730	0.47	0/981
2	H	0.26	0/1691	0.47	0/2301
3	L	0.26	0/1623	0.46	0/2215
All	All	0.26	0/4044	0.46	0/5497

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	710	638	634	2	0
2	H	1650	1565	1606	6	0
3	L	1583	1542	1542	1	0
4	A	17	0	0	0	0
4	H	17	0	0	0	0
4	L	17	0	0	0	0
All	All	3994	3745	3782	8	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 1.

The worst 5 of 8 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:66:ARG:NH2	2:H:89:ASP:OD2	2.32	0.62
2:H:138:THR:HB	2:H:142:THR:OG1	2.11	0.50
1:A:92:CYS:O	1:A:93:SER:CB	2.60	0.49
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.95	0.48
2:H:51:THR:O	2:H:51:THR:HG23	2.15	0.46

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	92/105 (88%)	91 (99%)	1 (1%)	0	100	100
2	H	215/238 (90%)	210 (98%)	5 (2%)	0	100	100
3	L	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
All	All	516/559 (92%)	503 (98%)	13 (2%)	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	83/93 (89%)	83 (100%)	0	100	100
2	H	184/199 (92%)	182 (99%)	2 (1%)	73	86
3	L	178/182 (98%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	445/474 (94%)	443 (100%)	2 (0%)	93 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	171[A]	HIS
2	H	171[B]	HIS

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 [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, 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	92/105 (87%)	0.77	10 (10%) 5 8	36, 51, 83, 94	0
2	H	218/238 (91%)	0.65	21 (9%) 8 10	36, 49, 81, 95	0
3	L	211/216 (97%)	0.62	22 (10%) 6 9	38, 51, 73, 88	0
All	All	521/559 (93%)	0.66	53 (10%) 6 9	36, 50, 81, 95	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	SER	5.5
3	L	213	THR	5.1
1	A	4[A]	GLN	4.9
1	A	70	SER	4.8
1	A	22	LEU	4.6

### 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.