

# wwPDB X-ray Structure Validation Summary Report (i)

#### Mar 11, 2024 – 12:33 PM JST

PDB ID : 8IQQ

Title : Crystal structure of Anti-PEG antibody M9 Fv-clasp fragment with PEG (co-

crystallization with PEG2000MME)

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Deposited on : 2023-03-17

Resolution : 2.02 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

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)

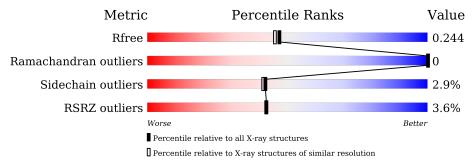
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.02 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	10434 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	L	179	91%		8%
1	1	179	91%	•	8%
2	Н	185	88%		8%
2	h	185	7% 90%		8%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6071 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.

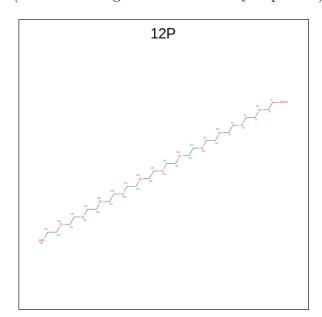
• Molecule 1 is a protein called M9 VL-SARAH.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	L	165	Total			0	S	0	1	0
			1316			252	8			
1	1	165	Total	С	N	O	$\mathbf{S}$	0	1	0
	1 1	100	1314	833	221	252	8		1	U

• Molecule 2 is a protein called M9 VH-SARAH.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			ZeroOcc	AltConf	Trace
2	П	171	Total	С	N	О	S	0	9	0
2	11	111	1364	864	220	270	10		2	U
2	h	171	Total	С	N	О	S	0	9	0
2	2   11	171	1368	868	220	271	9	0	Δ	0

• Molecule 3 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula:  $C_{24}H_{50}O_{13}$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	1	Total C O 37 24 13	0	0
3	h	1	Total C O 37 24 13	0	0

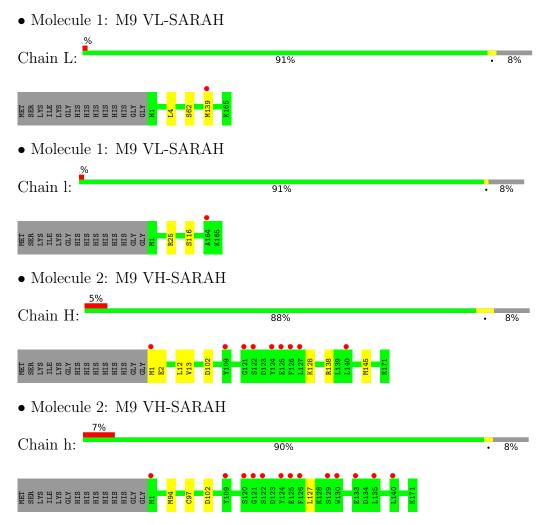
## $\bullet$ Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	148	Total O 148 148	0	0
4	Н	151	Total O 151 151	0	0
4	1	175	Total O 175 175	0	0
4	h	161	Total O 161 161	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.





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	109.99Å 70.25Å 103.58Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 110.94° 90.00°	Depositor
Resolution (Å)	48.37 - 2.02	Depositor
Resolution (A)	48.37 - 2.02	EDS
% Data completeness	99.8 (48.37-2.02)	Depositor
(in resolution range)	88.8 (48.37-2.02)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.63  (at  2.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
$R, R_{free}$	0.199 , 0.243	Depositor
It, It free	0.200 , 0.244	DCC
$R_{free}$ test set	2000 reflections $(4.13\%)$	wwPDB-VP
Wilson B-factor $(\mathring{A}^2)$	23.6	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 47.1	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 48.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5343e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: 12P

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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	L	0.25	0/1347	0.47	0/1817	
1	1	0.24	0/1345	0.47	0/1815	
2	Н	0.25	0/1400	0.49	0/1890	
2	h	0.25	0/1405	0.48	0/1898	
All	All	0.25	0/5497	0.48	0/7420	

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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	L	164/179 (92%)	160 (98%)	4 (2%)	0	100 100

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-	110111	DICULUUS	pauc

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	1	164/179 (92%)	159 (97%)	5 (3%)	0	100	100
2	Н	171/185 (92%)	166 (97%)	5 (3%)	0	100	100
2	h	171/185 (92%)	167 (98%)	4 (2%)	0	100	100
All	All	670/728 (92%)	652 (97%)	18 (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	L	148/158 (94%)	144 (97%)	4 (3%)		44	44
1	1	148/158 (94%)	146 (99%)	2 (1%)		67	70
2	Н	149/158 (94%)	141 (95%)	8 (5%)		22	17
2	h	149/158 (94%)	145 (97%)	4 (3%)		44	44
All	All	594/632 (94%)	576 (97%)	18 (3%)		42	40

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	h	94	MET
2	h	127	LEU
2	h	102	ASP
2	Н	102	ASP
1	1	116	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	19	GLN
2	Н	4	GLN
2	h	136	GLN



#### 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)

2 ligands are 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			
IVIOI	туре	Chain	rtes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	12P	h	201	-	36,36,36	0.55	0	35,35,35	0.20	0
3	12P	Н	201	-	36,36,36	0.55	0	35,35,35	0.20	0

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	12P	h	201	-	-	14/34/34/34	_
3	12P	Н	201	-	-	9/34/34/34	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

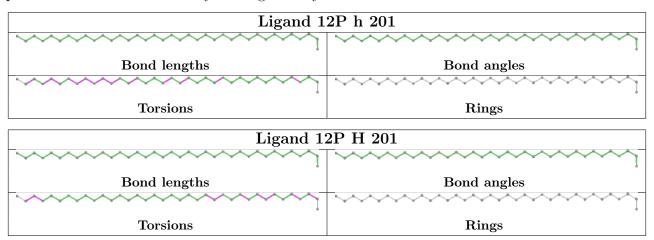


Mol	Chain	Res	Type	Atoms
3	Н	201	12P	O28-C29-C30-O31
3	h	201	12P	O4-C5-C6-O7
3	h	201	12P	O10-C11-C12-O13
3	Н	201	12P	O34-C35-C36-O37
3	h	201	12P	O13-C14-C15-O16

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



### 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,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	L	165/179~(92%)	-0.24	1 (0%) 89 89	21, 31, 49, 65	0
1	1	165/179~(92%)	-0.26	1 (0%) 89 89	20, 31, 54, 74	0
2	Н	171/185 (92%)	-0.02	9 (5%) 26 26	17, 29, 59, 79	0
2	h	171/185 (92%)	-0.06	13 (7%) 13 13	18, 29, 65, 74	0
All	All	672/728 (92%)	-0.14	24 (3%) 42 42	17, 31, 59, 79	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	122	SER	7.7
2	Н	121	GLY	5.9
2	Н	126	PHE	5.3
2	h	1	MET	4.9
2	h	124	TYR	4.2

### 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.

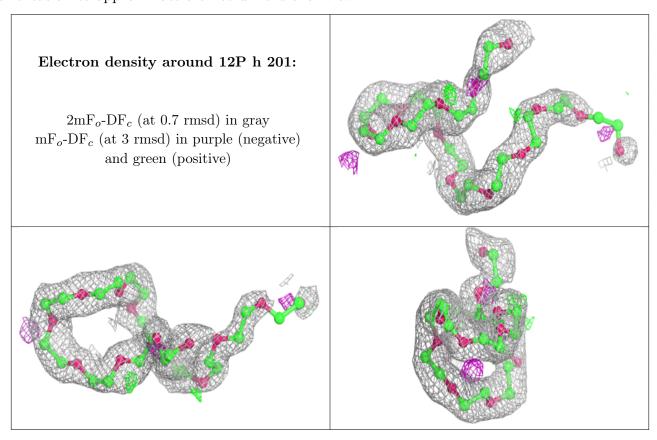
### 6.4 Ligands (i)

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,  $95^{th}$  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.

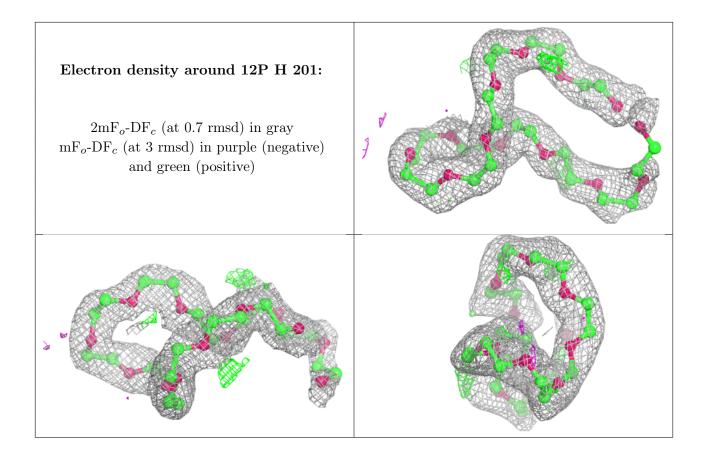


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	12P	h	201	37/37	0.86	0.17	23,39,59,65	0
3	12P	Н	201	37/37	0.90	0.16	22,37,57,69	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







# 6.5 Other polymers (i)

There are no such residues in this entry.

