

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

#### Oct 4, 2023 – 02:13 PM EDT

PDB ID	:	60BZ
Title	:	Crystal structure of FluA-20 Fab
Authors	:	Wilson, I.A.; Lang, S.
Deposited on		
Resolution	:	1.73  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:

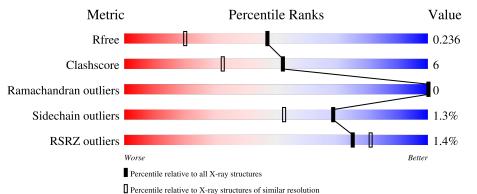
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.73 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3764(1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	А	235	% • 86%	9% 6%				
1	Н	235	% 82%	11% • 6%				
2	В	214	2% 90%	9%				
2	L	214	% 91%	8%				



#### 60BZ

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7648 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 Heavy chain of FluA-20 Fab.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	221	Total	С	Ν	Ο	S	0	0	0
	Л	221	1658	1048	272	331	7	0	0	0
1	Ц	221	Total	С	Ν	0	S	0	0	0
	11	221	1658	1048	272	331	7	0	0	0

• Molecule 2 is a protein called Light chain of FluA-20 Fab, Immunoglobulin light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
0	В	213	Total	С	Ν	Ο	S	0	0	0
	D	213	1646	1031	281	329	5	0	0	0
0	т	213	Total	С	Ν	0	S	0	0	0
	2 L	213	1646	1031	281	329	5		0	U

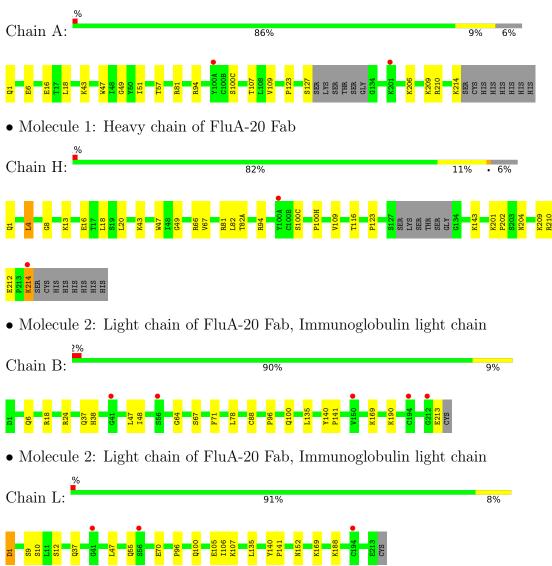
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	302	Total O 302 302	0	0
3	В	200	Total         O           200         200	0	0
3	Н	315	Total O 315 315	0	0
3	L	223	Total         O           223         223	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: Heavy chain of FluA-20 Fab



## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	83.58Å 52.64Å 104.79Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $93.77^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	50.00 - 1.73	Depositor	
Resolution (A)	45.67 - 1.72	EDS	
% Data completeness	96.5 (50.00-1.73)	Depositor	
(in resolution range)	96.6(45.67-1.72)	EDS	
R <sub>merge</sub>	(Not available)	Depositor	
R <sub>sym</sub>	0.10	Depositor	
$< I/\sigma(I) > 1$	$1.72 (at 1.73 \text{\AA})$	Xtriage	
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor	
D D.	0.202 , $0.238$	Depositor	
$R, R_{free}$	0.202 , $0.236$	DCC	
$R_{free}$ test set	4547 reflections $(4.89%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	15.7	Xtriage	
Anisotropy	0.265	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $47.7$	EDS	
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.46, \langle L^2 \rangle = 0.29$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.94	EDS	
Total number of atoms	7648	wwPDB-VP	
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



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

# 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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.45	0/1700	0.64	1/2325~(0.0%)	
1	Н	0.49	0/1700	0.65	2/2325~(0.1%)	
2	В	0.36	0/1683	0.57	0/2285	
2	L	0.38	0/1683	0.58	0/2285	
All	All	0.43	0/6766	0.61	3/9220~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Н	210	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	Н	4	LEU	CA-CB-CG	5.42	127.77	115.30
1	А	210	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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	А	1658	0	1615	19	0
1	Н	1658	0	1615	27	0
2	В	1646	0	1608	13	0
2	L	1646	0	1608	16	0
3	А	302	0	0	11	4
3	В	200	0	0	5	0

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001000	Continued from previous page										
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes					
3	Н	315	0	0	14	5					
3	L	223	0	0	8	1					
All	All	7648	0	6446	72	9					

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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 6.

The worst 5 of 72 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:H:81:ARG:NH1	3:H:302:HOH:O	1.96	0.99
2:L:100:GLN:NE2	3:L:301:HOH:O	2.03	0.91
1:A:127:SER:O	3:A:301:HOH:O	1.90	0.89
1:A:43:LYS:NZ	3:A:305:HOH:O	2.08	0.85
1:A:6:GLU:OE1	3:A:302:HOH:O	1.96	0.83

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:327:HOH:O	3:H:423:HOH:O[1_545]	1.70	0.50
3:H:321:HOH:O	3:H:327:HOH:O[2_658]	1.75	0.45
3:A:552:HOH:O	3:A:570:HOH:O[2_757]	1.93	0.27
3:A:594:HOH:O	3:L:497:HOH:O[1_564]	1.98	0.22
3:H:543:HOH:O	3:H:555:HOH:O[1_565]	2.03	0.17

### 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	А	217/235~(92%)	213~(98%)	4(2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Н	217/235~(92%)	213~(98%)	4 (2%)	0	100	100
2	В	211/214 (99%)	207~(98%)	4 (2%)	0	100	100
2	L	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
All	All	856/898~(95%)	840 (98%)	16 (2%)	0	100	100

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There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
1	А	192/205~(94%)	191 (100%)	1 (0%)	88	83
1	Н	192/205~(94%)	190~(99%)	2(1%)	76	63
2	В	189/190~(100%)	186~(98%)	3~(2%)	62	44
2	L	189/190~(100%)	185~(98%)	4 (2%)	53	30
All	All	762/790~(96%)	752~(99%)	10 (1%)	69	52

5 of 10 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	L	10	SER
2	L	135	LEU
2	L	152	ASN
2	В	190	LYS
1	Н	4	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
2	L	199	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)

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,  $95^{th}$  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	А	221/235~(94%)	0.30	2 (0%) 84 88	7, 14, 28, 41	0
1	Н	221/235~(94%)	0.33	2 (0%) 84 88	7, 14, 29, 37	0
2	В	213/214 (99%)	0.43	5 (2%) 60 66	10, 20, 35, 48	0
2	L	213/214 (99%)	0.36	3 (1%) 75 81	10, 18, 33, 47	0
All	All	868/898 (96%)	0.35	12 (1%) 75 81	7, 16, 33, 48	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	56	SER	3.2
1	Н	100(A)	TYR	3.0
2	В	212	GLY	2.8
1	Н	214	LYS	2.6
2	В	194	CYS	2.5

### 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.

