

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

#### Jun 13, 2024 – 01:29 PM EDT

PDB ID	:	1NBV
Title	:	AN AUTOANTIBODY TO SINGLE-STRANDED DNA: COMPARISON OF
		THE THREE-DIMENSIONAL STRUCTURES OF THE UNLIGANDED
		FAB AND A DEOXYNUCLEOTIDE-FAB COMPLEX
Authors	:	Herron, J.N.; He, X.M.; Edmundson, A.B.
Deposited on		
Resolution	:	2.00  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:

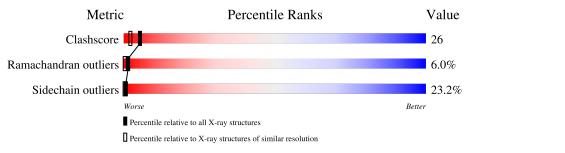
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
$\mathrm{EDS}$	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 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 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain						
1	L	219	38%	42%	15%	6%			
2	Н	219	32%	51%	11%	5%			



#### $1 \mathrm{NBV}$

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3347 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 IGG2B-KAPPA BV04-01 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	L	219	Total 1694	C 1056	N 289	O 342	S 7	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	39	HIS	TYR	CONFLICT	PIR S16112
L	51	LEU	PRO	CONFLICT	PIR S16112
L	55	LYS	ARG	CONFLICT	PIR S16112
L	94	SER	PHE	CONFLICT	PIR S16112
L	96	SER	GLY	CONFLICT	PIR S16112
L	101	LEU	TYR	CONFLICT	PIR S16112
L	105	ALA	GLY	CONFLICT	PIR S16112
L	108	LYS	ARG	CONFLICT	PIR S16112
L	111	LEU	ILE	CONFLICT	PIR S16112

• Molecule 2 is a protein called IGG2B-KAPPA BV04-01 FAB (HEAVY CHAIN).

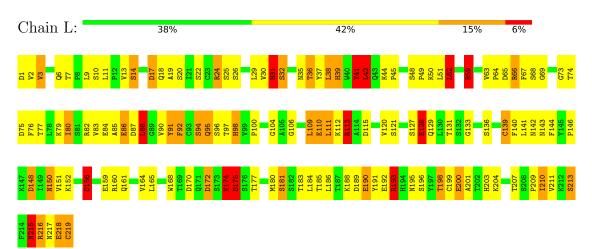
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Н	219	Total 1653	C 1038	N 275	O 330	S 10	0	0	0



# 3 Residue-property plots (i)

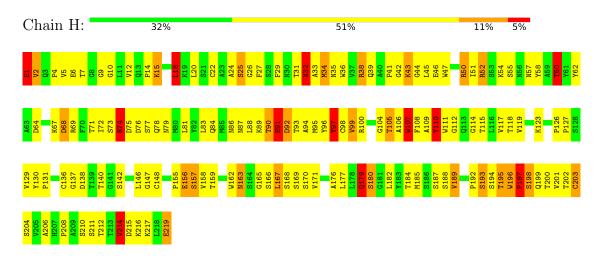
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.



• Molecule 1: IGG2B-KAPPA BV04-01 FAB (LIGHT CHAIN)

• Molecule 2: IGG2B-KAPPA BV04-01 FAB (HEAVY CHAIN)





## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	58.40Å 43.70Å 41.50Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$83.40^{\circ}$ $89.40^{\circ}$ $84.40^{\circ}$	Depositor	
Resolution (Å)	6.00 - 2.00	Depositor	
% Data completeness	(Not available) (6.00-2.00)	Depositor	
(in resolution range)	(1000 available) (0.00-2.00)	Depositor	
$R_{merge}$	(Not available)	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
Refinement program	PROLSQ, X-PLOR	Depositor	
$R, R_{free}$	0.246 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3347	wwPDB-VP	
Average B, all atoms $(Å^2)$	14.0	wwPDB-VP	



# 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	Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	L	1.24	7/1732~(0.4%)	1.79	51/2350~(2.2%)	
2	Н	1.20	6/1694~(0.4%)	1.77	30/2313~(1.3%)	
All	All	1.22	13/3426~(0.4%)	1.78	81/4663~(1.7%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Н	0	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	L	199	CYS	CB-SG	-9.35	1.66	1.82
1	L	128	GLU	CD-OE2	7.19	1.33	1.25
2	Н	91	GLU	CD-OE1	6.76	1.33	1.25
1	L	110	GLU	CD-OE2	6.53	1.32	1.25
2	Н	46	GLU	CD-OE2	6.46	1.32	1.25

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\mathbf{Ideal}(^{o})$
1	L	75	ASP	CB-CG-OD1	10.50	127.75	118.30
2	Н	156	GLU	CA-CB-CG	10.43	136.34	113.40
1	L	148	ASP	CB-CG-OD1	10.02	127.32	118.30
1	L	175	ASP	CB-CG-OD1	9.71	127.04	118.30
1	L	88	LEU	CA-CB-CG	9.55	137.27	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	Н	196	TRP	Mainchain

### 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	L	1694	0	1638	89	1
2	Н	1653	0	1600	98	1
All	All	3347	0	3238	173	1

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 26.

The worst 5 of 173 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:127:PRO:HD2	2:H:212:THR:HG21	1.50	0.91
1:L:1:ASP:HB2	1:L:100:PRO:HD2	1.59	0.84
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.58	0.83
2:H:22:CYS:HB3	2:H:81:LEU:HB3	1.62	0.80
1:L:95:GLN:HE21	1:L:97:THR:H	1.30	0.77

All (1) 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)
1:L:188:LYS:NZ	2:H:104:GLY:O[1_465]	2.18	0.02

## 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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	217/219~(99%)	183 (84%)	29~(13%)	5(2%)	6 2
2	Н	217/219 (99%)	166 (76%)	30 (14%)	21 (10%)	0 0
All	All	434/438~(99%)	349 (80%)	59 (14%)	26~(6%)	1 0

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	174	LYS
2	Н	2	VAL
2	Н	25	SER
2	Н	43	LYS
2	Н	107	TRP

#### 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	Percentiles
1	L	197/197~(100%)	149~(76%)	48 (24%)	0 0
2	Н	186/186 (100%)	145 (78%)	41 (22%)	1 0
All	All	383/383~(100%)	294 (77%)	89~(23%)	1 0

 $5~{\rm of}~89$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	Н	73	SER
2	Н	123	LYS
2	Н	83	LEU
2	Н	98	CYS
2	Н	155	PRO

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such side chains are listed below:



Mol	Chain	Res	Type
1	L	166	ASN
2	Н	32	ASN
2	Н	179	GLN
2	Н	86	ASN
1	L	98	HIS

#### 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

