

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

May 28, 2020 – 08:03 pm BST

PDB ID : 1NJ9

Title : Cocaine hydrolytic antibody 15A10

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Deposited on : 2002-12-30

Resolution : 2.35 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 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 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)

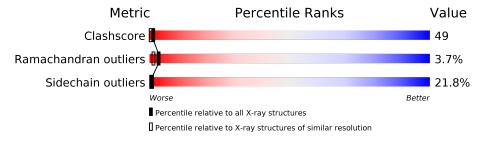
Validation Pipeline (wwPDB-VP) : 2.11

## 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 2.35 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	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$		
Clashscore	141614	$1232\ (2.36-2.36)$		
Ramachandran outliers	138981	1211 (2.36-2.36)		
Sidechain outliers	138945	1212 (2.36-2.36)		

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 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	A	212	31%	49%	20%				
1	L	212	24%	58%	16% •				
2	В	215	36%	50%	13% •				
2	Н	215	32%	51%	16%				



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6579 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 immunoglobulin variable chain.

	$\mathbf{Mol}$	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
	1	T	212	Total C N O S	0	0					
	1	П	212	1616	1010	271	329	6	0	U	U
Ī	1	Λ	212	Total	С	N	О	S	0	0	0
	1	Α	212	1616	1010	271	329	6	0	0	U

• Molecule 2 is a protein called immunoglobulin heavy chain.

Mol	Chain	Residues	${f Atoms}$					ZeroOcc	AltConf	Trace
2	Н	215	10001	C 1027	11	0	S 7	0	0	0
2	В	215	Total 1612	C 1020	N 265		S 7	0	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	3	Total Na 3 3	0	0
3	В	2	Total Na 2 2	0	0
3	A	1	Total Na 1 1	0	0
3	L	2	Total Na 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	25	Total O 25 25	0	0
4	Н	29	Total O 29 29	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	23	Total O 23 23	0	0
4	В	30	Total O 30 30	0	0

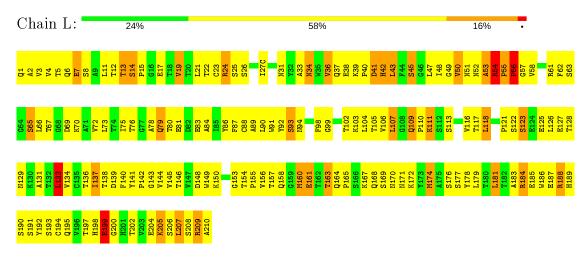


# 3 Residue-property plots (i)

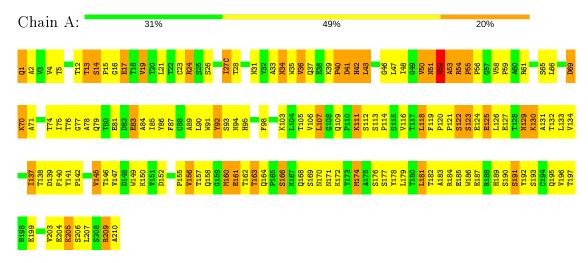
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



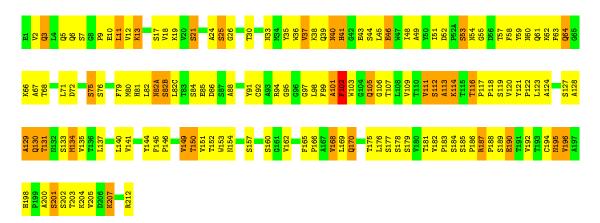
• Molecule 1: immunoglobulin variable chain



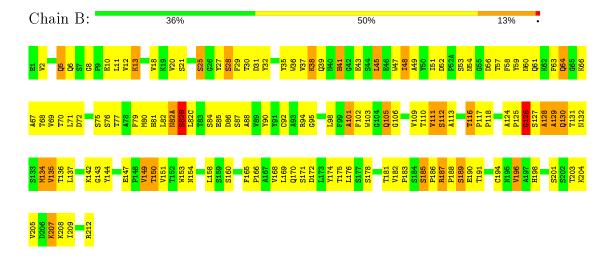
• Molecule 2: immunoglobulin heavy chain

Chain H: 32% 51% 16%





• Molecule 2: immunoglobulin 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 21 1	Depositor
Cell constants	37.50Å 108.40Å 111.30Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	30.00 - 2.35	Depositor
% Data completeness	80.0 (30.00-2.35)	Depositor
(in resolution range)	00.0 (80.00 2.88)	Беровног
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS 1.1, SHELXL-97 & CNS1.1	Depositor
$R, R_{free}$	0.199 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP



## 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: NA

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	Boı	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.44	0/1655	0.84	$3/2262 \ (0.1\%)$	
1	L	0.51	$1/1655 \ (0.1\%)$	1.03	$14/2262 \ (0.6\%)$	
2	В	0.45	0/1656	0.86	$2/2261 \ (0.1\%)$	
2	Н	0.50	0/1664	0.91	$2/2273 \ (0.1\%)$	
All	All	0.47	$1/6630 \ (0.0\%)$	0.91	21/9058 (0.2%)	

All (1) bond length outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type	Atoms	$\mathbf{Z}$	${f Observed(\AA)}$	$\operatorname{Ideal}( ext{\AA})$
1	L	55	PRO	CB-CG	-5.13	1.24	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathrm{Ideal}(^{o})$
1	L	55	PRO	N-CA-C	13.41	146.97	112.10
1	L	56	PRO	N-CA-C	-9.91	86.34	112.10
1	L	93	SER	CA-C-N	-9.21	96.93	117.20
2	В	126	GLY	N-CA-C	-8.72	91.30	113.10
1	L	93	SER	N-CA-C	8.61	134.23	111.00

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	1616	0	1556	181	0
1	L	1616	0	1556	161	0
2	В	1612	0	1552	160	0
2	Н	1620	0	1574	159	0
3	A	1	0	0	0	0
3	В	2	0	0	0	0
3	Н	3	0	0	0	0
3	L	2	0	0	0	0
4	A	23	0	0	4	0
4	В	30	0	0	6	0
4	Н	29	0	0	5	0
4	L	25	0	0	4	0
All	All	6579	0	6238	624	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 49.

The worst 5 of 624 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
1:L:2:ALA:HB1	1:L:26:SER:OG	1.34	1.24
1:L:54:ARG:HB3	1:L:55:PRO:HD3	1.21	1.12
1:L:45:SER:HB3	2:H:102:PHE:HE2	1.05	1.10
1:A:120:PRO:HG3	2:B:126:GLY:HA2	1.30	1.06
2:B:125:PRO:O	2:B:126:GLY:O	1.71	1.06

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	210/212 (99%)	185 (88%)	15 (7%)	10 (5%)	2 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	210/212 (99%)	188 (90%)	14 (7%)	8 (4%)	3 1
2	В	213/215 (99%)	182 (85%)	23 (11%)	8 (4%)	3 1
2	Н	213/215 (99%)	191 (90%)	17 (8%)	5 (2%)	6 4
All	All	846/854 (99%)	746 (88%)	69 (8%)	31 (4%)	3 1

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	160	MET
2	Н	129	ALA
1	A	41	ASP
1	A	160	MET
2	В	126	GLY

#### 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	Perce	entiles
1	A	183/183 (100%)	141 (77%)	42 (23%)	1	0
1	L	183/183 (100%)	139 (76%)	44 (24%)	0	0
2	В	181/184 (98%)	148 (82%)	33 (18%)	1	1
2	Н	184/184 (100%)	144 (78%)	40 (22%)	1	0
All	All	731/734 (100%)	572 (78%)	159 (22%)	1	0

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Н	150	THR
1	A	24	ARG
2	В	131	THR
2	Н	169	LEU
2	Н	195	ASN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	51	ASN
1	A	109	GLN
2	В	132	ASN
1	A	52	ASN
1	A	129	ASN

#### 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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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.

