



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2017 – 01:16 AM EDT

PDB ID : 1NJ9
Title : Cocaine hydrolytic antibody 15A10
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Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

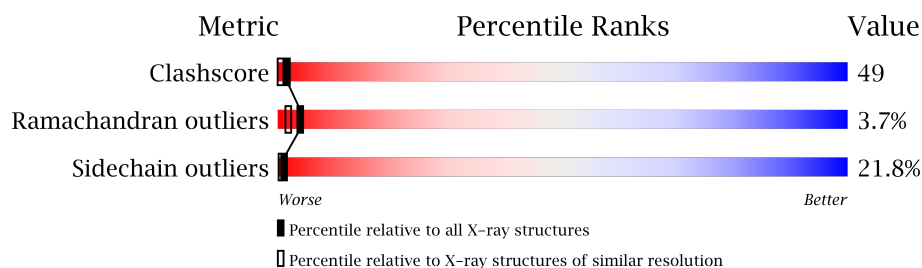
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	212	
1	L	212	
2	B	215	
2	H	215	

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1616	1010	271	329	6			
1	A	212	Total	C	N	O	S	0	0	0
			1616	1010	271	329	6			

- Molecule 2 is a protein called immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1620	1027	265	321	7			
2	B	215	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	3	Total	Na	0	0
			3	3		
3	B	2	Total	Na	0	0
			2	2		
3	A	1	Total	Na	0	0
			1	1		
3	L	2	Total	Na	0	0
			2	2		

- Molecule 4 is water.

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

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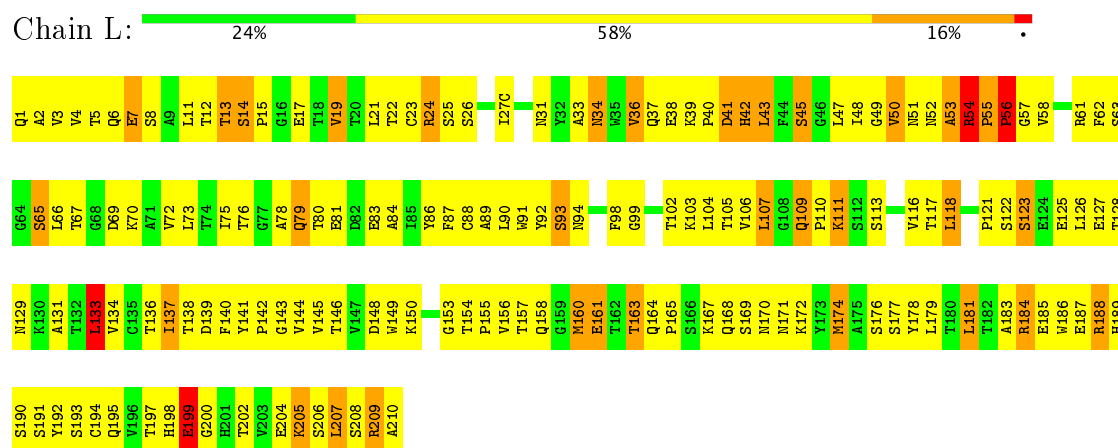
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	30	Total	O	0	0
			30	30		

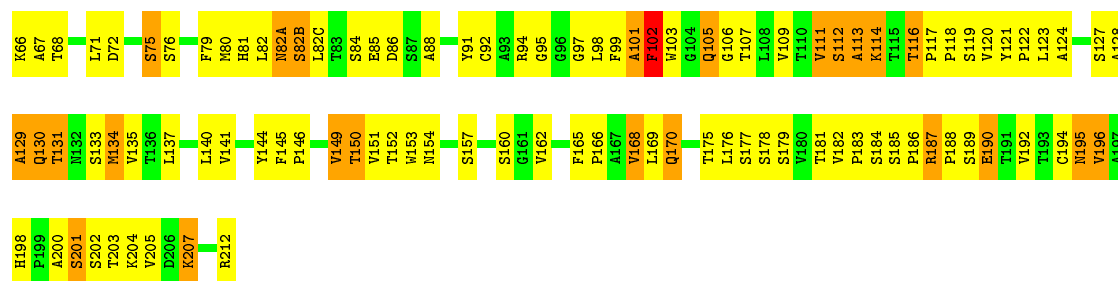
3 Residue-property plots [i](#)

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 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.

Note EDS was not executed.

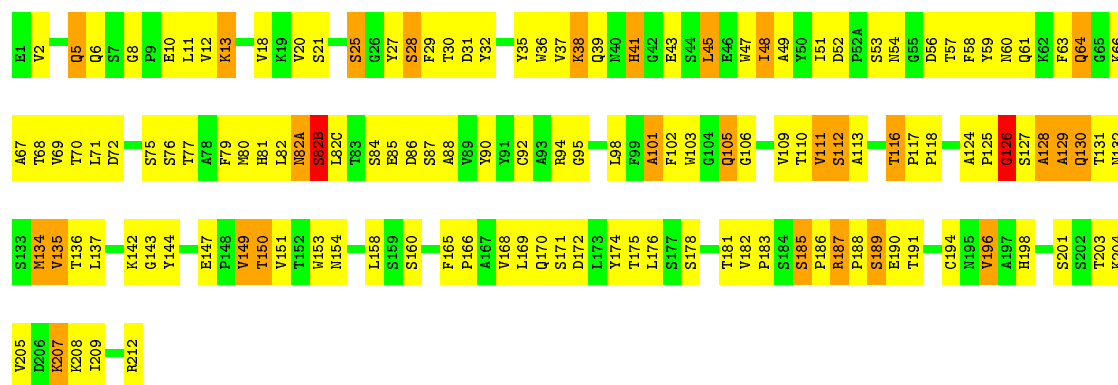
- Molecule 1: immunoglobulin variable chain





• Molecule 2: immunoglobulin heavy chain

Chain B: 36% 50% 13%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.50 Å 108.40 Å 111.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35	Depositor
% Data completeness (in resolution range)	80.0 (30.00-2.35)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	SHELXL-97 & CNS1.1, CNS 1.1	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 ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	Bond lengths		Bond angles	
		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	B	0.45	0/1656	0.86	2/2261 (0.1%)
2	H	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:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	Z	Observed(°)	Ideal(°)
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	B	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

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	B	1612	0	1552	160	0
2	H	1620	0	1574	159	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	H	3	0	0	0	0
3	L	2	0	0	0	0
4	A	23	0	0	4	0
4	B	30	0	0	6	0
4	H	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	Interatomic distance (Å)	Clash overlap (Å)
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 1

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

5 of 31 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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	183/183 (100%)	141 (77%)	42 (23%)	1	0
1	L	183/183 (100%)	139 (76%)	44 (24%)	1	0
2	B	181/184 (98%)	148 (82%)	33 (18%)	2	1
2	H	184/184 (100%)	144 (78%)	40 (22%)	1	1
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	H	150	THR
1	A	24	ARG
2	B	131	THR
2	H	169	LEU
2	H	195	ASN

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

Mol	Chain	Res	Type
1	A	51	ASN
1	A	109	GLN
2	B	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.