wwPDB X-ray Structure Validation Summary Report (i)

Oct 20, 2024 – 10:45 PM EDT

PDB ID	:	1NJ9
Title	:	Cocaine hydrolytic antibody 15A10
Authors	:	Larsen, N.A.; de Prada, P.; Deng, S.X.; Zhu, X.; Landry, D.W.; Wilson, I.A.
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

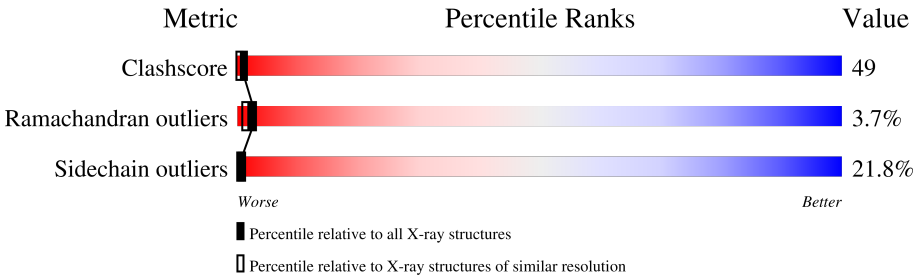
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (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 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	A	212	31% 49% 20%
1	L	212	24% 58% 16% •
2	B	215	36% 50% 13% •
2	H	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.

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	L	2	Total	Na	0	0
			2	2		
3	H	3	Total	Na	0	0
			3	3		
3	A	1	Total	Na	0	0
			1	1		
3	B	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 23 23	0	0
4	B	30	Total O 30 30	0	0

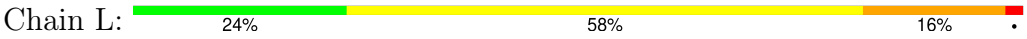
3 Residue-property plots (i)

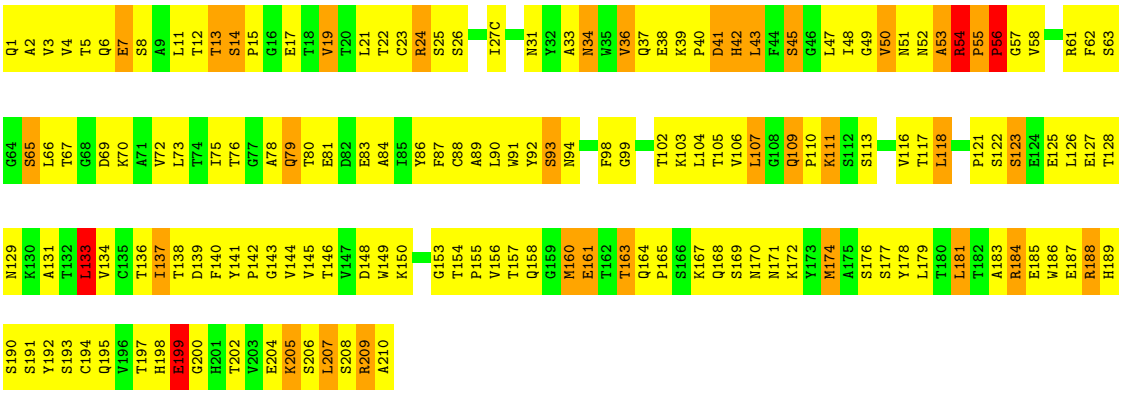
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

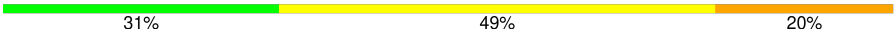
Chain L:

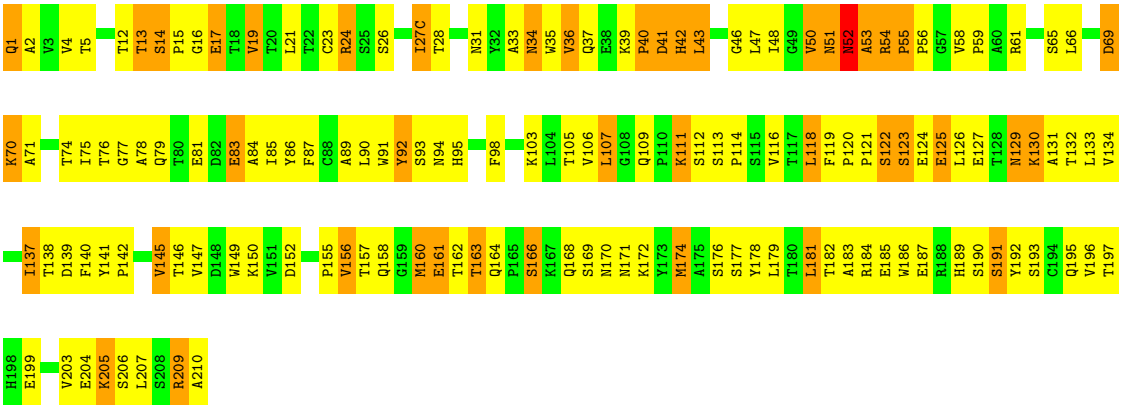




• Molecule 1: immunoglobulin variable chain

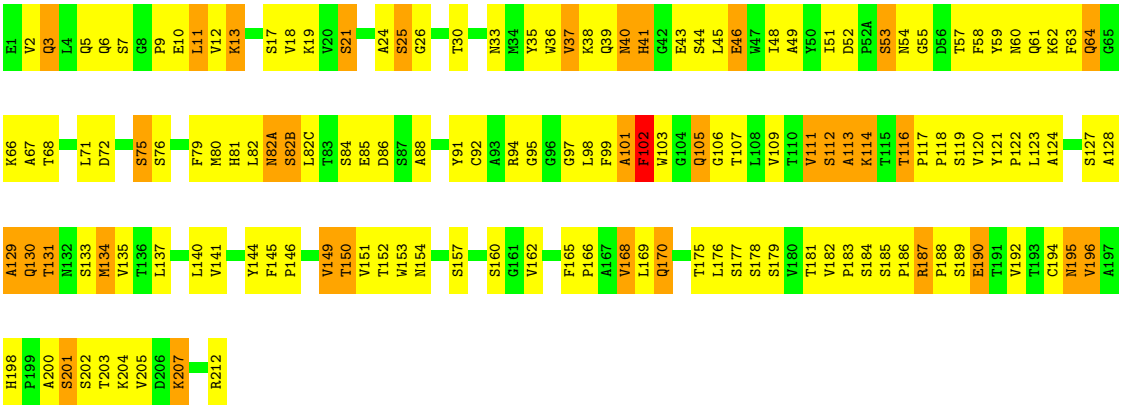
Chain A:





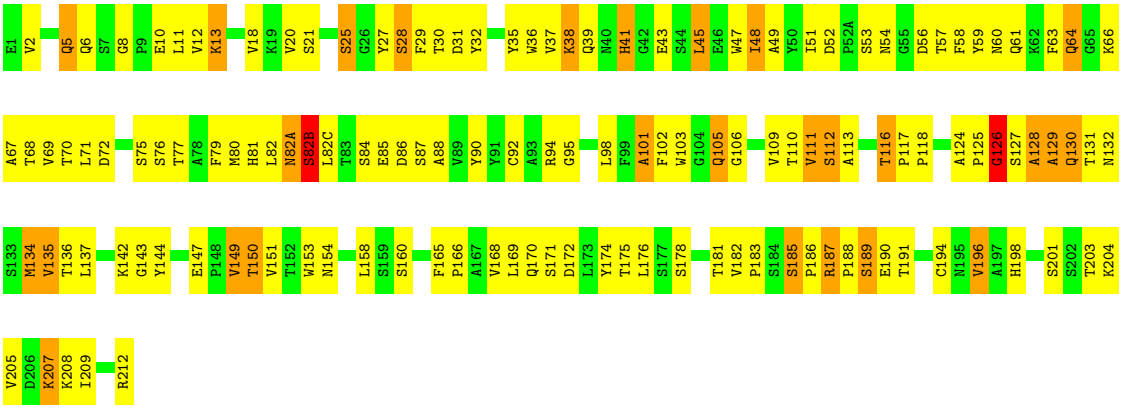
• Molecule 2: immunoglobulin heavy chain

Chain H:



• Molecule 2: immunoglobulin heavy chain

Chain B:



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 a, b, c, α, β, γ	37.50Å 108.40Å 111.30Å 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	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^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(^{o})	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	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 0

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

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 (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	A	183/183 (100%)	141 (77%)	42 (23%)	0	0
1	L	183/183 (100%)	139 (76%)	44 (24%)	0	0
2	B	181/184 (98%)	148 (82%)	33 (18%)	1	1
2	H	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
1	A	160	MET
2	B	111	VAL
1	A	169	SER
2	B	28	SER
2	B	150	THR

Sometimes 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	158	GLN
2	B	6	GLN
1	A	195	GLN
2	B	41	HIS
2	H	40	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 oligosaccharides 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

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.