wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 03:22 PM EDT

PDB ID	:	2NYY
Title	:	Crystal structure of botulinum neurotoxin type A complexed with monoclonal antibody CR1
Authors	:	Stevens, R.C.; Arndt, J.W.
Deposited on	:	2006-11-21
Resolution	:	2.61 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:

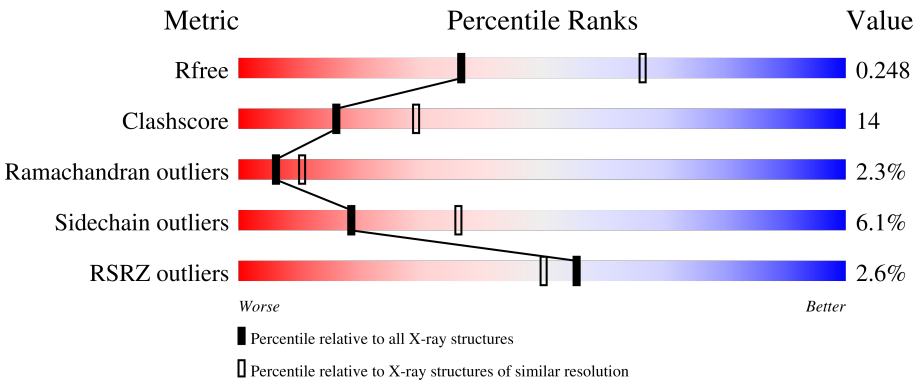
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.61 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))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	A	1295	3% 72% 21%
2	C	218	3% 72% 22%
3	D	223	2% 74% 19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13507 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1267	10211	6549	1691	1940	31	0	0	0

- Molecule 2 is a protein called CR1 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	216	1657	1039	279	334	5	0	0	0

- Molecule 3 is a protein called CR1 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	217	1637	1031	270	329	7	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

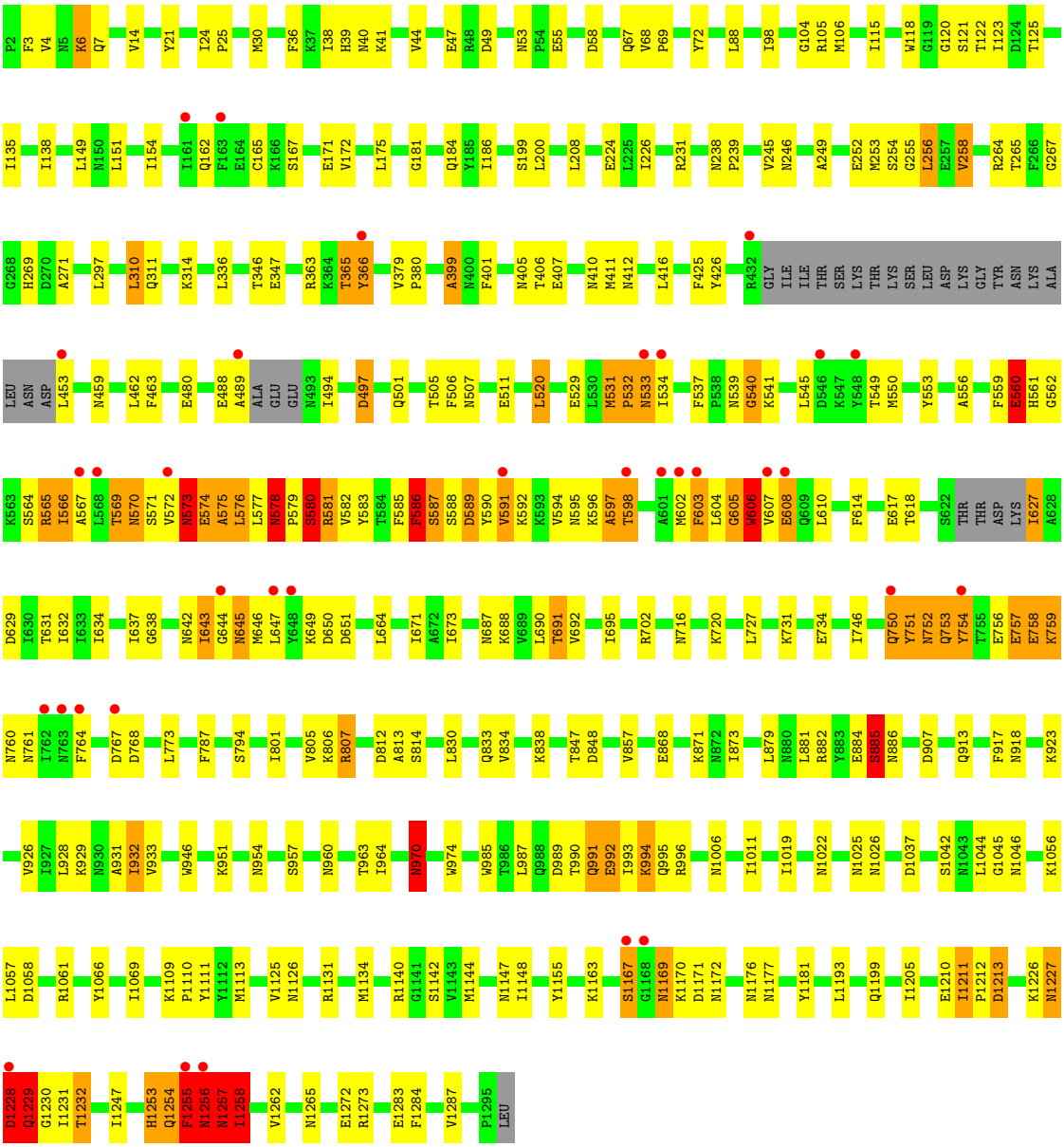
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0

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.

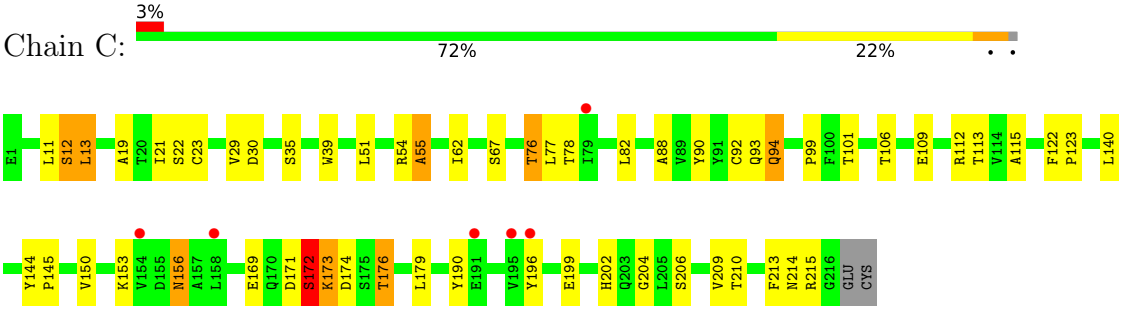
- Molecule 1: Botulinum neurotoxin type A

Chain A: 3% 72% 21%



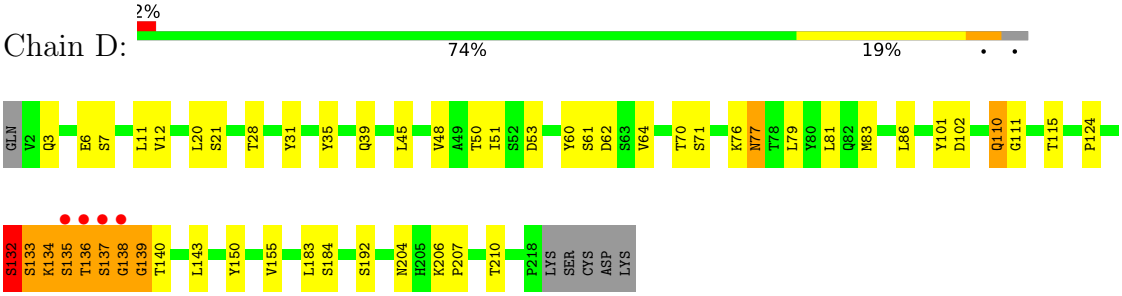
• Molecule 2: CR1 monoclonal antibody

Chain C:



• Molecule 3: CR1 monoclonal antibody

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.05Å 148.25Å 196.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 43.05 – 2.61	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.61) 89.4 (43.05-2.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.246 0.211 , 0.248	Depositor DCC
R_{free} test set	3912 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13507	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, ZN

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	0.64	0/10428	0.70	3/14115 (0.0%)
2	C	0.58	0/1695	0.67	0/2303
3	D	0.56	0/1678	0.65	0/2287
All	All	0.62	0/13801	0.69	3/18705 (0.0%)

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
1	A	0	46
2	C	0	2
3	D	0	5
All	All	0	53

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1140	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	1037	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	154	ILE	CB-CA-C	-5.03	101.55	111.60

There are no chirality outliers.

5 of 53 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	118	TRP	Peptide
1	A	532	PRO	Peptide
1	A	534	ILE	Peptide
1	A	6	LYS	Peptide

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	10211	0	10013	292	0
2	C	1657	0	1595	36	0
3	D	1637	0	1562	58	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
All	All	13507	0	13170	386	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 14.

The worst 5 of 386 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:A:578:ASN:HB3	1:A:579:PRO:C	1.38	1.43
1:A:1228:ASP:HB3	1:A:1229:GLN:CB	1.51	1.38
1:A:578:ASN:HB3	1:A:579:PRO:CA	1.48	1.33
3:D:139:GLY:N	3:D:140:THR:HB	1.40	1.32
1:A:604:LEU:N	1:A:605:GLY:HA3	1.55	1.15

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	1259/1295 (97%)	1112 (88%)	117 (9%)	30 (2%)	6	9
2	C	214/218 (98%)	198 (92%)	13 (6%)	3 (1%)	11	21
3	D	215/223 (96%)	193 (90%)	17 (8%)	5 (2%)	6	10
All	All	1688/1736 (97%)	1503 (89%)	147 (9%)	38 (2%)	6	10

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	560	GLU
1	A	566	ILE
1	A	576	LEU
1	A	578	ASN

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	1126/1178 (96%)	1055 (94%)	71 (6%)	18	35
2	C	186/190 (98%)	176 (95%)	10 (5%)	22	42
3	D	181/189 (96%)	171 (94%)	10 (6%)	21	41
All	All	1493/1557 (96%)	1402 (94%)	91 (6%)	18	36

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1042	SER
2	C	12	SER
1	A	1131	ARG
1	A	1227	ASN
2	C	94	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	970	ASN
1	A	1093	ASN
3	D	13	GLN
1	A	1006	ASN
1	A	1196	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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)

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, 95th 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	A	1267/1295 (97%)	-0.05	34 (2%)	54	49	2, 10, 33, 45	0
2	C	216/218 (99%)	0.05	6 (2%)	53	47	2, 14, 31, 38	0
3	D	217/223 (97%)	-0.16	4 (1%)	68	64	2, 17, 29, 30	0
All	All	1700/1736 (97%)	-0.05	44 (2%)	56	50	2, 11, 32, 45	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	754	TYR	5.4
1	A	489	ALA	4.9
1	A	603	PHE	4.7
3	D	136	THR	4.3
1	A	644	GLY	4.3

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	A	1297	1/1	0.58	0.13	63,63,63,63	0
4	ZN	A	1	1/1	0.99	0.04	3,3,3,3	0

6.5 Other polymers (i)

There are no such residues in this entry.