Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 05:47 PM EDT

PDB ID	:	3QW6
Title	:	Crystal structure of the protease domain of Botulinum Neurotoxin Serotype A with a peptide inhibitor RYGC
Authors	:	Kumaran, D.; Swaminathan, S.
Deposited on	:	2011-02-26
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

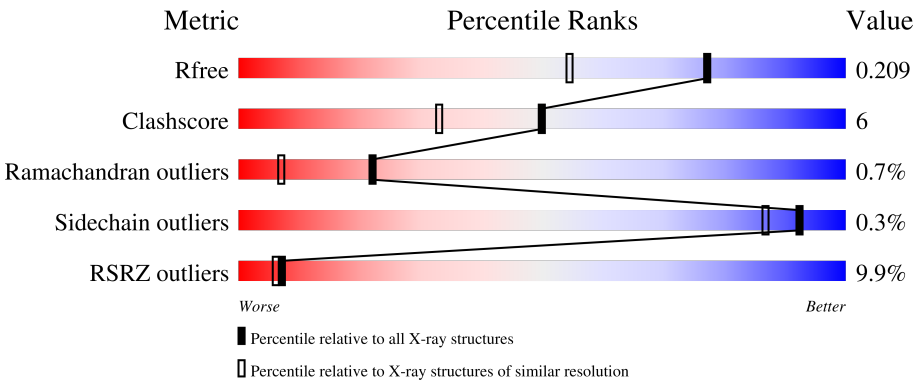
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	430	10% 87% 11% •
2	B	5	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3769 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	422	3415	2204	558	645	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	HIS	-	expression tag	UNP A5HZZ9
A	426	HIS	-	expression tag	UNP A5HZZ9
A	427	HIS	-	expression tag	UNP A5HZZ9
A	428	HIS	-	expression tag	UNP A5HZZ9
A	429	HIS	-	expression tag	UNP A5HZZ9
A	430	HIS	-	expression tag	UNP A5HZZ9

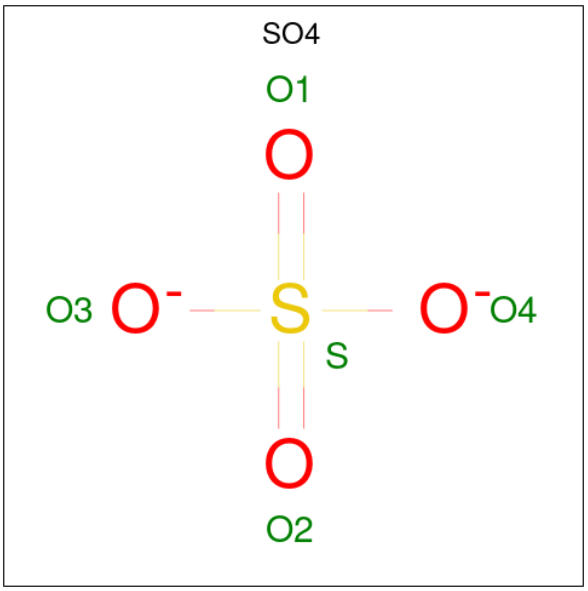
- Molecule 2 is a protein called inhibitory peptide RYGC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	5	34	20	8	5	1	0	0	1

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0

- Molecule 6 is water.

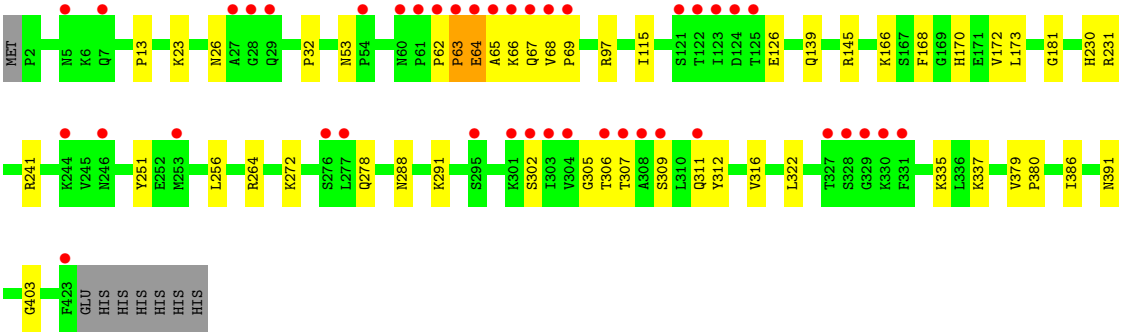
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	300	Total O 300 300	0	0
6	B	3	Total O 3 3	0	0

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.

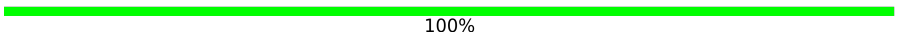
• Molecule 1: Botulinum neurotoxin type A

Chain A:



• Molecule 2: inhibitory peptide RYGC

Chain B:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.07Å 66.38Å 64.81Å 90.00° 98.38° 90.00°	Depositor
Resolution (Å)	35.99 – 1.60 35.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.0 (35.99-1.60) 90.7 (35.99-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.222 0.194 , 0.209	Depositor DCC
R_{free} test set	2606 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	1.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3769	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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: ZN, NH2, NA, SO4

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	0.33	0/3497	0.58	0/4734
2	B	0.48	0/33	0.50	0/42
All	All	0.33	0/3530	0.58	0/4776

There are no bond length outliers.

There are no bond angle outliers.

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	3415	0	3362	40	0
2	B	34	0	28	0	0
3	A	1	0	0	0	0
4	A	15	0	0	0	0
5	B	1	0	0	0	0
6	A	300	0	0	8	0
6	B	3	0	0	0	0
All	All	3769	0	3390	40	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 6.

All (40) 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:241:ARG:HH21	1:A:278:GLN:HE21	1.24	0.85
1:A:62:PRO:HB2	1:A:63:PRO:HD3	1.58	0.83
1:A:335:LYS:HE3	6:A:728:HOH:O	1.83	0.79
1:A:307:THR:HG22	6:A:764:HOH:O	1.82	0.77
1:A:139:GLN:NE2	1:A:145:ARG:HD3	2.00	0.76
1:A:139:GLN:HE21	1:A:145:ARG:HD3	1.56	0.71
1:A:306:THR:HG21	6:A:770:HOH:O	1.92	0.69
1:A:68:VAL:HG21	6:A:791:HOH:O	1.94	0.68
1:A:53:ASN:HB2	1:A:166:LYS:NZ	2.15	0.62
1:A:170:HIS:HD2	1:A:173:LEU:H	1.48	0.61
1:A:306:THR:HG23	6:A:819:HOH:O	2.02	0.59
1:A:311:GLN:HG2	1:A:312:TYR:N	2.20	0.57
1:A:251:TYR:HA	1:A:256:LEU:HD12	1.89	0.54
1:A:23:LYS:HE3	1:A:32:PRO:HG3	1.91	0.53
1:A:312:TYR:O	1:A:316:VAL:HG23	2.09	0.52
1:A:53:ASN:HB2	1:A:166:LYS:HZ1	1.73	0.52
1:A:272:LYS:HD2	6:A:817:HOH:O	2.09	0.52
1:A:62:PRO:HB2	1:A:63:PRO:CD	2.36	0.52
1:A:126:GLU:HG2	1:A:302:SER:OG	2.11	0.51
1:A:62:PRO:CB	1:A:63:PRO:HD3	2.33	0.49
1:A:391:ASN:HD22	1:A:403:GLY:H	1.61	0.48
1:A:170:HIS:CD2	1:A:172:VAL:H	2.31	0.48
1:A:68:VAL:HB	1:A:69:PRO:HD2	1.96	0.48
1:A:288:ASN:HA	1:A:291:LYS:HE2	1.96	0.48
1:A:230:HIS:CE1	1:A:264:ARG:HD3	2.49	0.47
1:A:241:ARG:NH2	1:A:278:GLN:HE21	2.01	0.47
1:A:309:SER:HB2	1:A:311:GLN:OE1	2.16	0.45
1:A:63:PRO:O	1:A:64:GLU:HB2	2.17	0.45
1:A:305:GLY:HA3	6:A:764:HOH:O	2.17	0.44
1:A:115:ILE:HD12	1:A:316:VAL:HG11	2.00	0.44
1:A:115:ILE:HD12	1:A:316:VAL:CG1	2.49	0.43
1:A:166:LYS:HE2	1:A:166:LYS:HB3	1.74	0.43
1:A:181:GLY:HA2	1:A:231:ARG:O	2.18	0.42
1:A:379:VAL:HB	1:A:380:PRO:HD3	2.02	0.42
1:A:97:ARG:HA	1:A:386:ILE:HG23	2.01	0.42
1:A:26:ASN:HA	1:A:168:PHE:CE1	2.54	0.41
1:A:13:PRO:HG2	6:A:826:HOH:O	2.20	0.41
1:A:66:LYS:NZ	1:A:66:LYS:HB3	2.35	0.41
1:A:63:PRO:HB2	1:A:64:GLU:H	1.60	0.41
1:A:322:LEU:O	1:A:337:LYS:HE2	2.21	0.40

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	420/430 (98%)	404 (96%)	13 (3%)	3 (1%)	22 7
2	B	3/5 (60%)	3 (100%)	0	0	100 100
All	All	423/435 (97%)	407 (96%)	13 (3%)	3 (1%)	22 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	64	GLU
1	A	65	ALA

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	377/385 (98%)	376 (100%)	1 (0%)	92 87
2	B	3/3 (100%)	3 (100%)	0	100 100
All	All	380/388 (98%)	379 (100%)	1 (0%)	92 87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	9	ASN
1	A	29	GLN
1	A	67	GLN
1	A	139	GLN
1	A	170	HIS
1	A	174	ASN
1	A	278	GLN
1	A	391	ASN
1	A	394	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	503	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	A	502	-	4,4,4	0.25	0	6,6,6	0.05	0

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	422/430 (98%)	0.52	42 (9%) 7 6	10, 19, 45, 62	0
2	B	4/5 (80%)	0.66	0 100 100	21, 22, 26, 27	0
All	All	426/435 (97%)	0.52	42 (9%) 7 6	10, 19, 45, 62	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ALA	14.4
1	A	62	PRO	10.8
1	A	327	THR	10.2
1	A	27	ALA	8.7
1	A	67	GLN	7.9
1	A	303	ILE	7.8
1	A	329	GLY	7.3
1	A	63	PRO	7.3
1	A	66	LYS	7.0
1	A	68	VAL	6.3
1	A	64	GLU	6.2
1	A	328	SER	5.9
1	A	125	THR	5.8
1	A	61	PRO	5.7
1	A	277	LEU	5.5
1	A	307	THR	4.6
1	A	28	GLY	4.5
1	A	122	THR	4.2
1	A	301	LYS	4.2
1	A	123	ILE	4.1
1	A	302	SER	4.1
1	A	308	ALA	3.8
1	A	7	GLN	3.8
1	A	311	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	304	VAL	3.5
1	A	244	LYS	3.3
1	A	54	PRO	3.1
1	A	121	SER	3.0
1	A	423	PHE	2.9
1	A	253	MET	2.8
1	A	124	ASP	2.8
1	A	29	GLN	2.8
1	A	331	PHE	2.6
1	A	276	SER	2.6
1	A	309	SER	2.5
1	A	246	ASN	2.3
1	A	330	LYS	2.3
1	A	60	ASN	2.3
1	A	5	ASN	2.3
1	A	306	THR	2.3
1	A	295	SER	2.1
1	A	69	PRO	2.1

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
4	SO4	A	504	5/5	0.88	0.27	51,51,52,53	0
4	SO4	A	502	5/5	0.94	0.10	47,47,48,48	0
5	NA	B	301	1/1	0.96	0.19	35,35,35,35	0
4	SO4	A	503	5/5	0.98	0.07	25,29,30,31	0
3	ZN	A	501	1/1	1.00	0.04	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.