



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:57 PM GMT

PDB ID : 1Z7H
Title : 2.3 Angstrom crystal structure of tetanus neurotoxin light chain
Authors : Breidenbach, M.A.; Brunger, A.T.
Deposited on : 2005-03-24
Resolution : 2.30 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

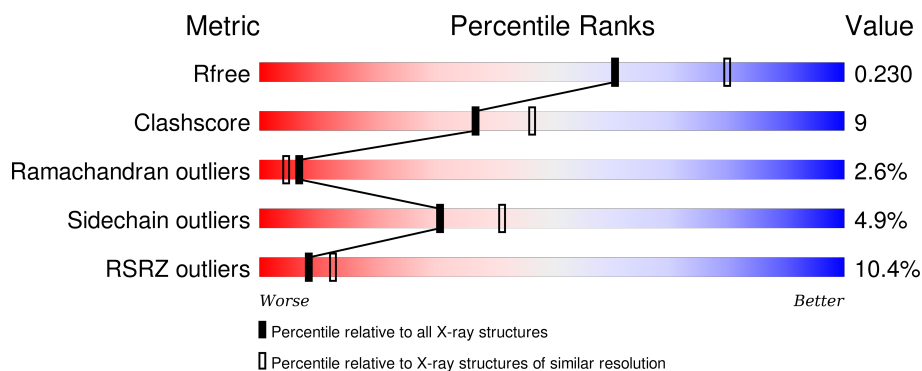
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	447	<div> <div>9%</div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3783 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 Tetanus toxin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	174	0	0
			3453	2206	560	671	16			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	cloning artifact	UNP P04958
A	-2	SER	-	cloning artifact	UNP P04958
A	-1	HIS	-	cloning artifact	UNP P04958
A	0	MET	-	cloning artifact	UNP P04958
A	361	VAL	ILE	ENGINEERED	UNP P04958

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

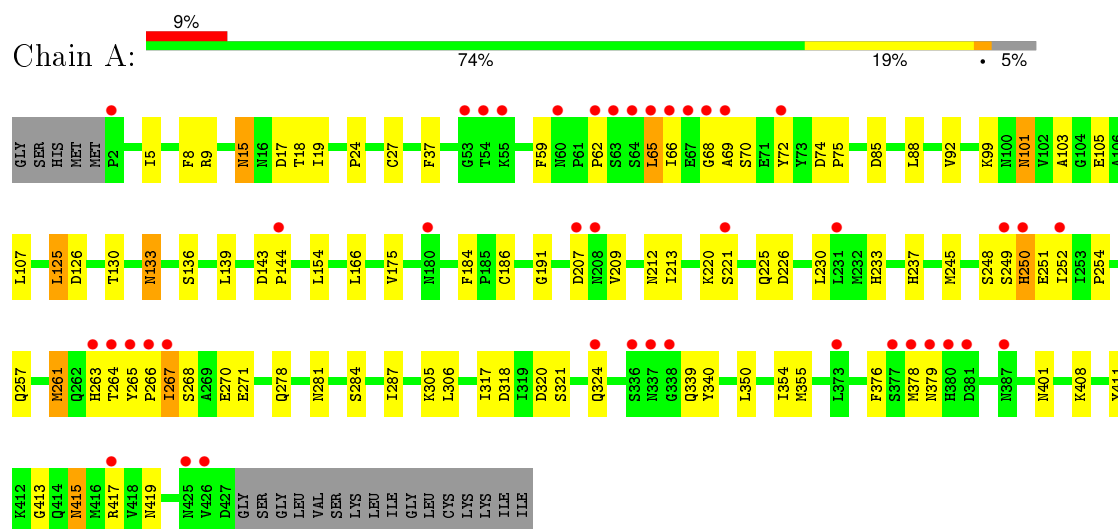
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	328	Total	O	0	0
			328	328		

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 errors 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 ($\text{RSRZ} > 2$). 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: Tetanus toxin light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.35Å 176.86Å 57.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.76 – 2.30 38.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.76-2.30) 99.8 (38.76-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.88 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.216 0.221 , 0.230	Depositor DCC
R_{free} test set	2354 reflections (9.74%)	DCC
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.916	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 45855 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3783	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.37	0/3532	0.63	0/4785

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	3453	0	3368	61	0
2	A	2	0	0	0	0
3	A	328	0	0	2	1
All	All	3783	0	3368	61	1

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 9.

All (61) 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:267:ILE:HG13	1:A:268:SER:H	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:HB3	1:A:267:ILE:O	1.83	0.78
1:A:15:ASN:HD22	1:A:17:ASP:H	1.37	0.70
1:A:15:ASN:HD21	1:A:19:ILE:H	1.40	0.69
1:A:101:ASN:HD22	1:A:103:ALA:H	1.42	0.67
1:A:74:ASP:HB3	1:A:166:LEU:HD11	1.78	0.66
1:A:225:GLN:HE21	1:A:226:ASP:H	1.43	0.65
1:A:175:VAL:HG22	1:A:184:PHE:CE2	2.34	0.63
1:A:267:ILE:HG13	1:A:268:SER:N	2.08	0.63
1:A:15:ASN:ND2	1:A:17:ASP:H	1.97	0.61
1:A:278:GLN:NE2	1:A:281:ASN:HD22	1.98	0.61
1:A:415:ASN:HD22	1:A:417:ARG:H	1.52	0.57
1:A:225:GLN:NE2	1:A:226:ASP:H	2.03	0.55
1:A:101:ASN:ND2	1:A:103:ALA:H	2.05	0.55
1:A:15:ASN:C	1:A:15:ASN:HD22	2.10	0.54
1:A:136:SER:OG	1:A:154:LEU:HD23	2.08	0.54
1:A:59:PHE:O	1:A:75:PRO:HG3	2.09	0.53
1:A:24:PRO:HG2	1:A:27:CYS:SG	2.50	0.52
1:A:62:PRO:HG3	1:A:65:LEU:HD13	1.91	0.52
1:A:15:ASN:ND2	1:A:19:ILE:H	2.08	0.51
1:A:72:TYR:CD2	1:A:166:LEU:HD12	2.46	0.50
1:A:237:HIS:CE1	1:A:270:GLU:HG3	2.46	0.50
1:A:350:LEU:O	1:A:354:ILE:HG12	2.12	0.49
1:A:320:ASP:O	1:A:324:GLN:HG2	2.10	0.49
1:A:378:MET:HG2	1:A:379:ASN:N	2.28	0.49
1:A:65:LEU:HG	1:A:66:ILE:O	2.13	0.49
1:A:250:HIS:NE2	1:A:287:ILE:HG23	2.27	0.49
1:A:263:HIS:CG	1:A:264:THR:N	2.80	0.48
1:A:250:HIS:CD2	1:A:287:ILE:HG23	2.49	0.47
1:A:88:LEU:O	1:A:92:VAL:HG23	2.14	0.47
1:A:401:ASN:HD22	1:A:413:GLY:HA3	1.79	0.47
1:A:250:HIS:O	1:A:251:GLU:HB2	2.15	0.47
1:A:245:MET:HE2	1:A:355:MET:SD	2.54	0.47
1:A:125:LEU:HD13	1:A:126:ASP:N	2.29	0.47
1:A:5:ILE:HG12	1:A:99:LYS:HD3	1.96	0.47
1:A:125:LEU:HA	1:A:305:LYS:HE3	1.98	0.46
1:A:415:ASN:ND2	1:A:417:ARG:H	2.13	0.45
1:A:130:THR:HG21	1:A:317:ILE:HD12	1.98	0.45
1:A:15:ASN:HD21	1:A:18:THR:N	2.13	0.45
1:A:15:ASN:HD21	1:A:18:THR:H	1.63	0.45
1:A:324:GLN:NE2	3:A:485:HOH:O	2.50	0.44
1:A:68:GLY:O	1:A:70:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HG	1:A:66:ILE:N	2.32	0.44
1:A:186:CYS:HA	1:A:191:GLY:HA2	2.00	0.44
1:A:284:SER:HB2	3:A:690:HOH:O	2.17	0.42
1:A:101:ASN:HD22	1:A:103:ALA:N	2.13	0.42
1:A:230:LEU:O	1:A:233:HIS:HB3	2.20	0.42
1:A:267:ILE:CG1	1:A:268:SER:H	2.13	0.42
1:A:248:SER:O	1:A:249:SER:C	2.59	0.42
1:A:130:THR:HG21	1:A:317:ILE:CD1	2.50	0.41
1:A:133:ASN:HD22	1:A:133:ASN:N	2.18	0.41
1:A:378:MET:HG2	1:A:379:ASN:H	1.84	0.41
1:A:265:TYR:O	1:A:376:PHE:HE1	2.03	0.41
1:A:263:HIS:CD2	1:A:264:THR:N	2.89	0.41
1:A:401:ASN:HB3	1:A:408:LYS:HA	2.02	0.41
1:A:318:ASP:HB3	1:A:321:SER:HB3	2.03	0.41
1:A:9:ARG:NH2	1:A:85:ASP:OD2	2.55	0.40
1:A:37:PHE:CD1	1:A:37:PHE:N	2.89	0.40
1:A:415:ASN:C	1:A:415:ASN:HD22	2.24	0.40
1:A:268:SER:OG	1:A:271:GLU:HG2	2.21	0.40
1:A:339:GLN:HG3	1:A:340:TYR:N	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:738:HOH:O	3:A:738:HOH:O 3_656	2.11	0.09

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	424/447 (95%)	387 (91%)	26 (6%)	11 (3%)	7 4

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	221	SER
1	A	257	GLN
1	A	252	ILE
1	A	69	ALA
1	A	144	PRO
1	A	261	MET
1	A	267	ILE
1	A	250	HIS
1	A	254	PRO
1	A	209	VAL

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	391/408 (96%)	372 (95%)	19 (5%)	31	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	15	ASN
1	A	101	ASN
1	A	105	GLU
1	A	107	LEU
1	A	125	LEU
1	A	133	ASN
1	A	139	LEU
1	A	143	ASP
1	A	207	ASP
1	A	212	ASN
1	A	213	ILE
1	A	220	LYS
1	A	261	MET

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Mol	Chain	Res	Type
1	A	266	PRO
1	A	306	LEU
1	A	411	TYR
1	A	415	ASN
1	A	419	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	15	ASN
1	A	100	ASN
1	A	101	ASN
1	A	131	ASN
1	A	133	ASN
1	A	225	GLN
1	A	278	GLN
1	A	304	ASN
1	A	324	GLN
1	A	401	ASN
1	A	415	ASN
1	A	419	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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	404/447 (90%)	0.56	42 (10%) 8 12	12, 26, 76, 102	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	ASN	11.3
1	A	63	SER	9.7
1	A	65	LEU	9.5
1	A	265	TYR	8.9
1	A	378	MET	8.2
1	A	263	HIS	7.7
1	A	66	ILE	7.5
1	A	69	ALA	7.2
1	A	208	ASN	5.4
1	A	64	SER	5.3
1	A	62	PRO	5.1
1	A	221	SER	5.1
1	A	264	THR	4.9
1	A	377	SER	4.5
1	A	252	ILE	4.5
1	A	249	SER	4.1
1	A	266	PRO	4.1
1	A	267	ILE	4.0
1	A	324	GLN	4.0
1	A	68	GLY	3.9
1	A	53	GLY	3.8
1	A	250	HIS	3.5
1	A	381	ASP	3.5
1	A	72	TYR	3.3
1	A	426	VAL	3.1
1	A	180	ASN	3.1
1	A	373	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	67	GLU	3.0
1	A	380	HIS	3.0
1	A	417	ARG	3.0
1	A	425	ASN	3.0
1	A	387	ASN	2.7
1	A	2	PRO	2.7
1	A	336	SER	2.6
1	A	144	PRO	2.4
1	A	207	ASP	2.4
1	A	54	THR	2.3
1	A	55	LYS	2.3
1	A	231	LEU	2.3
1	A	60	ASN	2.2
1	A	337	ASN	2.0
1	A	338	GLY	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	A	445	1/1	0.98	0.11	-1.82	22,22,22,22	0
2	ZN	A	444	1/1	0.81	0.56	-	95,95,95,95	1

6.5 Other polymers [i](#)

There are no such residues in this entry.