



Full wwPDB X-ray Structure Validation Report

Dec 22, 2020 – 09:03 am GMT

PDB ID : 7AE8
Title : Crystal structure of HEPN(R102A) toxin
Authors : Tamulaitiene, G.; Sasnauskas, G.; Songailiene, I.; Juozapaitis, J.; Siksnyis, V.
Deposited on : 2020-09-17
Resolution : 2.00 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  symbol.

The following versions of software and data (see [references](#) ) 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 : 2.16
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) : 2.16

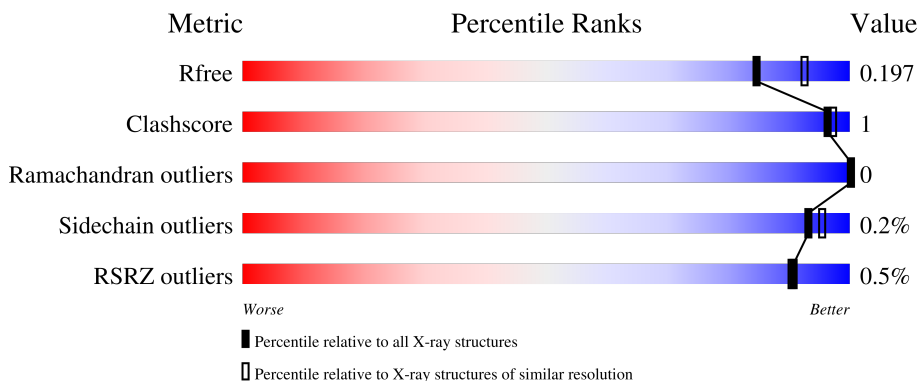
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

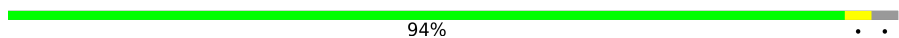
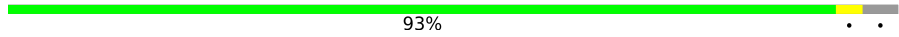


The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	157	94% 
1	B	157	93% 
1	C	157	88% 
1	D	157	92% 

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5091 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 HEPN toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1267	808	207	251	1	0	5	0
1	B	150	1266	807	208	250	1	0	6	0
1	C	142	1191	768	198	224	1	0	5	0
1	D	148	1177	756	186	233	2	0	1	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0B0QJR1
A	2	THR	-	expression tag	UNP A0A0B0QJR1
A	3	ASN	-	expression tag	UNP A0A0B0QJR1
A	4	ILE	-	expression tag	UNP A0A0B0QJR1
A	102	ALA	ARG	engineered mutation	UNP A0A0B0QJR1
A	148	LEU	-	expression tag	UNP A0A0B0QJR1
A	149	GLU	-	expression tag	UNP A0A0B0QJR1
A	150	SER	-	expression tag	UNP A0A0B0QJR1
A	151	GLY	-	expression tag	UNP A0A0B0QJR1
A	152	HIS	-	expression tag	UNP A0A0B0QJR1
A	153	HIS	-	expression tag	UNP A0A0B0QJR1
A	154	HIS	-	expression tag	UNP A0A0B0QJR1
A	155	HIS	-	expression tag	UNP A0A0B0QJR1
A	156	HIS	-	expression tag	UNP A0A0B0QJR1
A	157	HIS	-	expression tag	UNP A0A0B0QJR1
B	1	MET	-	initiating methionine	UNP A0A0B0QJR1
B	2	THR	-	expression tag	UNP A0A0B0QJR1
B	3	ASN	-	expression tag	UNP A0A0B0QJR1
B	4	ILE	-	expression tag	UNP A0A0B0QJR1
B	102	ALA	ARG	engineered mutation	UNP A0A0B0QJR1
B	148	LEU	-	expression tag	UNP A0A0B0QJR1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	149	GLU	-	expression tag	UNP A0A0B0QJR1
B	150	SER	-	expression tag	UNP A0A0B0QJR1
B	151	GLY	-	expression tag	UNP A0A0B0QJR1
B	152	HIS	-	expression tag	UNP A0A0B0QJR1
B	153	HIS	-	expression tag	UNP A0A0B0QJR1
B	154	HIS	-	expression tag	UNP A0A0B0QJR1
B	155	HIS	-	expression tag	UNP A0A0B0QJR1
B	156	HIS	-	expression tag	UNP A0A0B0QJR1
B	157	HIS	-	expression tag	UNP A0A0B0QJR1
C	1	MET	-	initiating methionine	UNP A0A0B0QJR1
C	2	THR	-	expression tag	UNP A0A0B0QJR1
C	3	ASN	-	expression tag	UNP A0A0B0QJR1
C	4	ILE	-	expression tag	UNP A0A0B0QJR1
C	102	ALA	ARG	engineered mutation	UNP A0A0B0QJR1
C	148	LEU	-	expression tag	UNP A0A0B0QJR1
C	149	GLU	-	expression tag	UNP A0A0B0QJR1
C	150	SER	-	expression tag	UNP A0A0B0QJR1
C	151	GLY	-	expression tag	UNP A0A0B0QJR1
C	152	HIS	-	expression tag	UNP A0A0B0QJR1
C	153	HIS	-	expression tag	UNP A0A0B0QJR1
C	154	HIS	-	expression tag	UNP A0A0B0QJR1
C	155	HIS	-	expression tag	UNP A0A0B0QJR1
C	156	HIS	-	expression tag	UNP A0A0B0QJR1
C	157	HIS	-	expression tag	UNP A0A0B0QJR1
D	1	MET	-	initiating methionine	UNP A0A0B0QJR1
D	2	THR	-	expression tag	UNP A0A0B0QJR1
D	3	ASN	-	expression tag	UNP A0A0B0QJR1
D	4	ILE	-	expression tag	UNP A0A0B0QJR1
D	102	ALA	ARG	engineered mutation	UNP A0A0B0QJR1
D	148	LEU	-	expression tag	UNP A0A0B0QJR1
D	149	GLU	-	expression tag	UNP A0A0B0QJR1
D	150	SER	-	expression tag	UNP A0A0B0QJR1
D	151	GLY	-	expression tag	UNP A0A0B0QJR1
D	152	HIS	-	expression tag	UNP A0A0B0QJR1
D	153	HIS	-	expression tag	UNP A0A0B0QJR1
D	154	HIS	-	expression tag	UNP A0A0B0QJR1
D	155	HIS	-	expression tag	UNP A0A0B0QJR1
D	156	HIS	-	expression tag	UNP A0A0B0QJR1
D	157	HIS	-	expression tag	UNP A0A0B0QJR1

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 63 63	0	0
3	B	53	Total O 53 53	0	0
3	C	25	Total O 25 25	0	0
3	D	37	Total O 37 37	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: HEPN toxin

Chain A:  94%

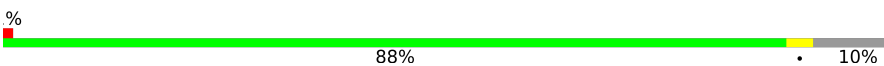


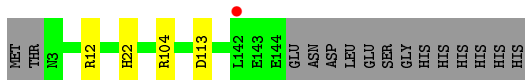
- Molecule 1: HEPN toxin

Chain B:  93%



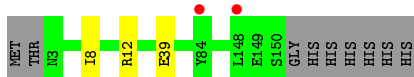
- Molecule 1: HEPN toxin

Chain C:  88% 10%



- Molecule 1: HEPN toxin

Chain D:  92% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.90Å 69.78Å 81.51Å 90.00° 107.01° 90.00°	Depositor
Resolution (Å)	51.99 – 2.00 51.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.99-2.00) 100.0 (51.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.73 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.169 , 0.195 0.171 , 0.197	Depositor DCC
R_{free} test set	4532 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtrriage
Anisotropy	0.247	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5091	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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, 0.333 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: ACT

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	0.25	0/1290	0.39	0/1751
1	B	0.25	0/1287	0.39	0/1743
1	C	0.24	0/1213	0.38	0/1645
1	D	0.25	0/1198	0.37	0/1631
All	All	0.25	0/4988	0.38	0/6770

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	1267	0	1227	4	0
1	B	1266	0	1243	2	0
1	C	1191	0	1180	3	0
1	D	1177	0	1126	2	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	D	4	0	3	0	0
3	A	63	0	0	1	0
3	B	53	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	25	0	0	0	0
3	D	37	0	0	0	0
All	All	5091	0	4785	10	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 1.

All (10) 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:B:3:ASN:HB2	1:B:65:LYS:HG3	1.78	0.65
1:A:3[B]:ASN:N	1:A:3[B]:ASN:OD1	2.32	0.58
1:C:104[A]:ARG:HH21	1:C:113:ASP:H	1.54	0.56
1:C:22[B]:HIS:CE1	1:D:39:GLU:HG2	2.46	0.51
1:A:104:ARG:HE	2:A:201:ACT:H2	1.76	0.51
1:D:8:ILE:O	1:D:12:ARG:HG2	2.11	0.50
1:C:104[A]:ARG:NH2	1:C:113:ASP:H	2.10	0.50
1:B:8:ILE:O	1:B:12[B]:ARG:HG2	2.14	0.47
1:A:4:ILE:HA	1:A:65:LYS:HG3	1.96	0.46
1:A:14[A]:GLU:HG3	3:A:336:HOH:O	2.19	0.42

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	155/157 (99%)	152 (98%)	3 (2%)	0	100	100
1	B	154/157 (98%)	151 (98%)	3 (2%)	0	100	100
1	C	145/157 (92%)	142 (98%)	3 (2%)	0	100	100
1	D	147/157 (94%)	144 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	601/628 (96%)	589 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	140/144 (97%)	140 (100%)	0	100	100
1	B	140/144 (97%)	140 (100%)	0	100	100
1	C	129/144 (90%)	127 (98%)	2 (2%)	62	67
1	D	126/144 (88%)	126 (100%)	0	100	100
All	All	535/576 (93%)	533 (100%)	2 (0%)	93	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12[A]	ARG
1	C	12[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

3 ligands are modelled in this entry.

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
2	ACT	A	201	-	1,3,3	6.72	1 (100%)	0,3,3	0.00	-
2	ACT	B	201	-	1,3,3	6.30	1 (100%)	0,3,3	0.00	-
2	ACT	D	201	-	1,3,3	6.98	1 (100%)	0,3,3	0.00	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	ACT	CH3-C	6.98	1.57	1.48
2	A	201	ACT	CH3-C	6.72	1.57	1.48
2	B	201	ACT	CH3-C	6.30	1.56	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	ACT	1	0

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 [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	152/157 (96%)	-0.34	0 100 100	22, 35, 61, 90	0
1	B	150/157 (95%)	-0.40	0 100 100	21, 36, 60, 85	0
1	C	142/157 (90%)	-0.19	1 (0%) 87 87	25, 40, 62, 84	0
1	D	148/157 (94%)	-0.12	2 (1%) 75 74	24, 40, 72, 88	0
All	All	592/628 (94%)	-0.27	3 (0%) 91 90	21, 38, 63, 90	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	148	LEU	2.2
1	C	142	LEU	2.2
1	D	84	TYR	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(\AA^2)	Q<0.9
2	ACT	D	201	4/4	0.83	0.18	52,53,55,56	0
2	ACT	B	201	4/4	0.86	0.14	38,45,49,50	0
2	ACT	A	201	4/4	0.86	0.17	40,44,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.