



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2022 – 10:05 pm BST

PDB ID : 7QHI  
Title : Crystal structure of cytotoxin 13 from Naja naja, hexagonal form  
Authors : Samygina, V.R.; Dubova, K.M.; Bourenkov, G.; Utkin, Y.N.; Dubovskii, P.V.  
Deposited on : 2021-12-12  
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](mailto: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  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

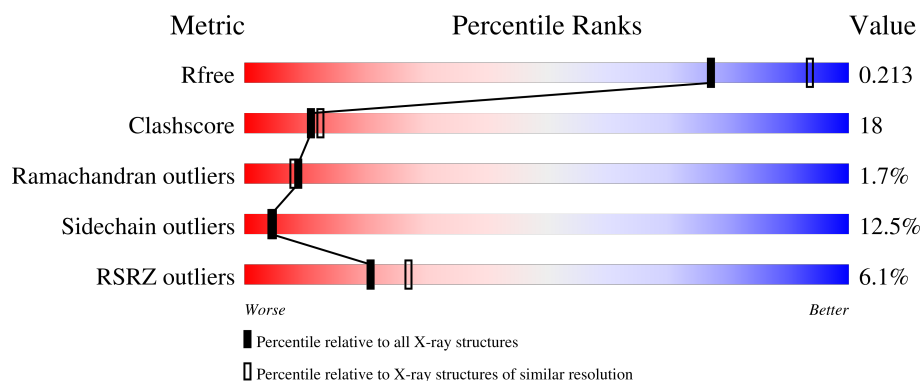
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AAA	72	<div> <div>14%</div> <div>64% 11% 8% 17%</div> </div>
1	BBB	72	<div> <div>62% 18% 17%</div> </div>
1	CCC	72	<div> <div>14%</div> <div>47% 26% 10% 17%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1609 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 Cytotoxin 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			
1	BBB	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			
1	CCC	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			

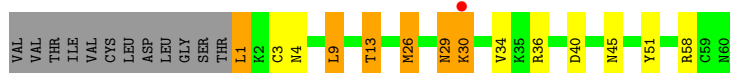
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	91	Total	O	0	0
			91	91		
2	BBB	76	Total	O	0	0
			76	76		
2	CCC	50	Total	O	0	0
			50	50		

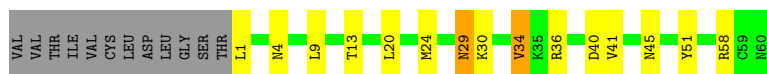
### 3 Residue-property plots [i](#)

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: Cytotoxin 13



- Molecule 1: Cytotoxin 13



- Molecule 1: Cytotoxin 13



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.33Å 109.33Å 135.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.90 – 2.30 14.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (14.90-2.30) 98.9 (14.95-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.43 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.199 , 0.228 0.203 , 0.213	Depositor DCC
$R_{free}$ test set	1084 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	AAA	0.72	0/471	1.02	0/632
1	BBB	0.73	0/471	1.12	2/632 (0.3%)
1	CCC	0.76	0/471	1.15	2/632 (0.3%)
All	All	0.73	0/1413	1.10	4/1896 (0.2%)

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	CCC	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	36	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	BBB	36	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	CCC	36	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	CCC	36	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	53	CYS	Peptide

## 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	AAA	464	0	492	22	0
1	BBB	464	0	492	14	0
1	CCC	464	0	492	21	0
2	AAA	91	0	0	9	0
2	BBB	76	0	0	6	0
2	CCC	50	0	0	3	0
All	All	1609	0	1476	52	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 18.

All (52) 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:BBB:9:LEU:CD1	2:BBB:139:HOH:O	2.26	0.84
1:BBB:4:ASN:HD21	1:BBB:58:ARG:HE	1.29	0.81
1:BBB:9:LEU:HD12	2:BBB:139:HOH:O	1.81	0.80
1:AAA:4:ASN:HD21	1:AAA:58:ARG:HE	1.32	0.74
1:AAA:9:LEU:HD21	1:BBB:34:VAL:HG13	1.68	0.74
1:CCC:20:LEU:HD23	1:CCC:40:ASP:O	1.88	0.73
1:AAA:40:ASP:HB3	2:AAA:124:HOH:O	1.88	0.73
1:BBB:45:ASN:HD21	1:BBB:51:TYR:H	1.40	0.70
1:AAA:13:THR:HG22	2:AAA:172:HOH:O	1.97	0.65
1:AAA:9:LEU:HD11	1:BBB:34:VAL:CG1	2.30	0.61
1:BBB:45:ASN:ND2	1:BBB:51:TYR:H	1.98	0.61
1:BBB:40:ASP:HB3	2:BBB:134:HOH:O	2.00	0.60
1:CCC:30:LYS:O	1:CCC:31:THR:O	2.21	0.58
1:AAA:45:ASN:ND2	1:AAA:51:TYR:H	2.02	0.57
1:BBB:29:ASN:C	1:BBB:29:ASN:HD22	2.08	0.57
1:AAA:9:LEU:HD23	1:CCC:27:VAL:HG22	1.87	0.56
1:CCC:23:LYS:NZ	2:CCC:102:HOH:O	2.38	0.56
2:AAA:159:HOH:O	1:CCC:27:VAL:CG1	2.54	0.56
1:AAA:45:ASN:HD21	1:AAA:51:TYR:H	1.54	0.55
1:CCC:32:VAL:HA	2:CCC:103:HOH:O	2.07	0.55
1:AAA:4:ASN:ND2	1:AAA:58:ARG:HE	2.02	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:3:CYS:SG	1:CCC:14:CYS:SG	3.06	0.52
1:CCC:31:THR:HG22	2:CCC:114:HOH:O	2.11	0.51
1:CCC:4:ASN:HD21	1:CCC:58:ARG:HE	1.59	0.51
1:AAA:29:ASN:ND2	1:AAA:30:LYS:HE2	2.26	0.50
1:CCC:26:MET:C	1:CCC:27:VAL:HG23	2.33	0.49
1:AAA:9:LEU:HD11	1:BBB:34:VAL:HG12	1.93	0.49
2:AAA:159:HOH:O	1:CCC:27:VAL:HG12	2.12	0.48
1:AAA:29:ASN:HD21	1:AAA:30:LYS:CE	2.25	0.48
2:AAA:159:HOH:O	1:CCC:27:VAL:HG11	2.14	0.48
1:AAA:29:ASN:ND2	1:AAA:30:LYS:CE	2.78	0.47
1:BBB:9:LEU:HD13	2:BBB:139:HOH:O	2.05	0.47
1:CCC:1:LEU:HD12	1:CCC:19:ASN:HA	1.97	0.46
1:CCC:45:ASN:ND2	1:CCC:51:TYR:H	2.14	0.46
1:BBB:24:MET:HE1	2:BBB:160:HOH:O	2.15	0.46
1:CCC:4:ASN:ND2	1:CCC:58:ARG:HE	2.14	0.46
1:AAA:1:LEU:HD13	1:AAA:3:CYS:SG	2.56	0.45
1:AAA:36:ARG:NH2	2:AAA:101:HOH:O	2.43	0.45
1:AAA:36:ARG:NH1	2:AAA:101:HOH:O	2.17	0.45
1:AAA:29:ASN:C	1:AAA:29:ASN:HD22	2.20	0.44
1:AAA:13:THR:CG2	2:AAA:172:HOH:O	2.60	0.43
2:BBB:155:HOH:O	1:CCC:27:VAL:HG21	2.18	0.42
1:AAA:26:MET:HE3	1:AAA:26:MET:HB2	1.94	0.42
1:CCC:19:ASN:C	1:CCC:20:LEU:HD22	2.40	0.42
1:BBB:29:ASN:HD22	1:BBB:30:LYS:N	2.18	0.42
1:CCC:29:ASN:O	1:CCC:30:LYS:O	2.38	0.42
1:CCC:43:PRO:HG2	1:CCC:51:TYR:CE1	2.55	0.41
1:CCC:29:ASN:C	1:CCC:30:LYS:O	2.58	0.41
1:AAA:9:LEU:CD2	1:BBB:34:VAL:HG13	2.44	0.41
1:AAA:26:MET:HA	1:AAA:26:MET:HE2	2.01	0.41
1:AAA:36:ARG:CZ	2:AAA:101:HOH:O	2.64	0.41
1:CCC:56:THR:HB	1:CCC:59:CYS:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	AAA	58/72 (81%)	55 (95%)	3 (5%)	0	100	100
1	BBB	58/72 (81%)	57 (98%)	1 (2%)	0	100	100
1	CCC	58/72 (81%)	51 (88%)	4 (7%)	3 (5%)	2	1
All	All	174/216 (81%)	163 (94%)	8 (5%)	3 (2%)	9	8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	27	VAL
1	CCC	30	LYS
1	CCC	31	THR

### 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	AAA	56/67 (84%)	49 (88%)	7 (12%)	4	5
1	BBB	56/67 (84%)	50 (89%)	6 (11%)	6	7
1	CCC	56/67 (84%)	48 (86%)	8 (14%)	3	3
All	All	168/201 (84%)	147 (88%)	21 (12%)	4	5

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1	LEU
1	AAA	9	LEU
1	AAA	13	THR
1	AAA	26	MET
1	AAA	29	ASN
1	AAA	30	LYS
1	AAA	34	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	BBB	1	LEU
1	BBB	13	THR
1	BBB	20	LEU
1	BBB	29	ASN
1	BBB	34	VAL
1	BBB	41	VAL
1	CCC	1	LEU
1	CCC	13	THR
1	CCC	23	LYS
1	CCC	28	SER
1	CCC	29	ASN
1	CCC	34	VAL
1	CCC	41	VAL
1	CCC	56	THR

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](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	60/72 (83%)	0.04	1 (1%) 70 76	26, 37, 52, 64	0
1	BBB	60/72 (83%)	-0.21	0 100 100	23, 33, 46, 60	0
1	CCC	60/72 (83%)	0.77	10 (16%) 1 2	25, 54, 87, 97	0
All	All	180/216 (83%)	0.20	11 (6%) 21 27	23, 37, 79, 97	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	16	ALA	5.4
1	CCC	29	ASN	4.4
1	CCC	17	GLY	4.1
1	CCC	54	CYS	4.0
1	CCC	55	ASN	3.2
1	CCC	13	THR	2.8
1	CCC	41	VAL	2.8
1	CCC	56	THR	2.5
1	CCC	21	CYS	2.5
1	CCC	1	LEU	2.4
1	AAA	30	LYS	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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.