



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 05:12 pm GMT

PDB ID : 4V1D  
Title : Ternary complex among two human derived single chain antibody fragments and Cn2 toxin from scorpion *Centruroides noxi*.  
Authors : Riano-Umbarila, L.; Serrano-Posada, H.; Rojas-Trejo, S.; Rudino-Pinera, E.; Becerril, B.  
Deposited on : 2014-09-25  
Resolution : 3.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

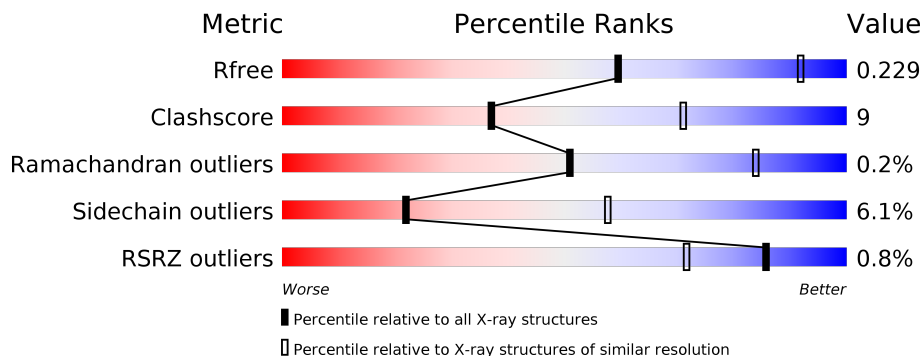
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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  $\geq 3$ , 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	117	<div> <div style="width: 87%;"></div> <div style="width: 13%;"></div> </div>
2	B	146	<div> <div style="width: 60%;"></div> <div style="width: 14%;"></div> <div style="width: 25%;"></div> </div>
3	C	66	<div> <div style="width: 2%;"></div> <div style="width: 77%;"></div> <div style="width: 21%;"></div> </div>
4	D	124	<div> <div style="width: 80%;"></div> <div style="width: 17%;"></div> </div>
5	E	149	<div> <div style="width: 50%;"></div> <div style="width: 21%;"></div> <div style="width: 25%;"></div> </div>







- Molecule 1: SINGLE CHAIN ANTIBODY FRAGMENT LR, HEAVY CHAIN

E1	V2	Q13	L20	F27	T28	F29	M34	I58	D59	Y60	K65	F68	L79	M83	T91	T106	T114	S117
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Category	Count
K1	16
E2	15
V6	14
D7	13
K8	12
N9	11
T10	10
G11	9
C12	8
K18	7
L26	6
K30	5
Y42	4
T49	3
W58	2
P59	1
L60	1
P61	1
N62	1
C65	1
S66	1

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GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	S139	N140	T144	P153	T158	I159	S162	N167	R177	H178	L179	L186	I187	I188	N192	R193	P195	S196	G197	P198	P199	D200	R201	F202	S203	A204	T215	L218	Q219	D222	E223	A224	P232
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S234	L235	L236	L246	T247	V248	L249	G250	ALA	ALA	ALA	GLU	GLN	LYS	LEU	ILE	SER	GLU	GLU	ASP	LEU	ASN	GLY	ALA	ALA	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.58Å 74.64Å 140.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.21 – 3.10 38.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.21-3.10) 99.9 (38.90-3.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.69 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.185 , 0.229 0.184 , 0.229	Depositor DCC
$R_{free}$ test set	438 reflections (4.77%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4046	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.28	0/911	0.54	0/1227
2	B	0.34	0/866	0.61	0/1175
3	C	0.36	1/538 (0.2%)	0.59	0/725
4	D	0.23	0/975	0.46	0/1316
5	E	0.51	1/841 (0.1%)	0.65	0/1146
All	All	0.35	2/4131 (0.0%)	0.57	0/5589

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
5	E	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	249	LEU	C-N	-5.45	1.23	1.33
3	C	65	CYS	C-N	-5.20	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	194	ARG	Peptide
5	E	199	PRO	Peptide
5	E	233	ASP	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	A	894	0	850	9	0
2	B	847	0	825	13	1
3	C	524	0	492	8	0
4	D	953	0	913	13	1
5	E	822	0	772	30	0
6	A	3	0	0	0	0
6	D	1	0	0	0	0
6	E	2	0	0	0	0
All	All	4046	0	3852	70	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.

The worst 5 of 70 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)
3:C:62:ASN:ND2	5:E:234:SER:OG	1.97	0.97
1:A:58:ILE:O	3:C:18:LYS:NZ	2.22	0.73
5:E:193:GLN:HG2	5:E:193:GLN:O	1.88	0.72
5:E:200:ASP:C	5:E:202:PHE:H	1.91	0.68
5:E:200:ASP:O	5:E:202:PHE:N	2.26	0.67

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)
2:B:148:GLY:O	4:D:17:SER:OG[2_667]	2.18	0.02



5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	119	LEU
5	E	158	THR
5	E	218	LEU
4	D	121	THR
2	B	224[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	62	ASN
5	E	193	GLN

### 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](#)

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 [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, 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	A	117/117 (100%)	-0.45	0 100 100	30, 43, 68, 93	0
2	B	109/146 (74%)	-0.36	0 100 100	30, 46, 62, 73	0
3	C	66/66 (100%)	-0.63	1 (1%) 74 54	27, 39, 60, 94	0
4	D	124/124 (100%)	-0.50	1 (0%) 86 71	32, 47, 65, 87	0
5	E	112/149 (75%)	-0.30	2 (1%) 69 47	31, 43, 71, 82	0
All	All	528/602 (87%)	-0.44	4 (0%) 86 71	27, 45, 68, 94	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	192	ASN	2.7
5	E	196	SER	2.5
3	C	66	SER	2.1
4	D	1	GLN	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](#)

There are no ligands in this entry.

