



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 12:18 pm GMT

PDB ID : 1UMR
Title : Crystal structure of the platelet activator convulxin, a disulfide linked a4b4 cyclic tetramer from the venom of *Crotalus durissus terrificus*
Authors : Murakami, M.T.; Zela, S.P.; Gava, L.M.; Michelin-Duarte, S.; Cintra, A.C.O.; Arni, R.K.
Deposited on : 2003-08-28
Resolution : 2.40 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

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
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

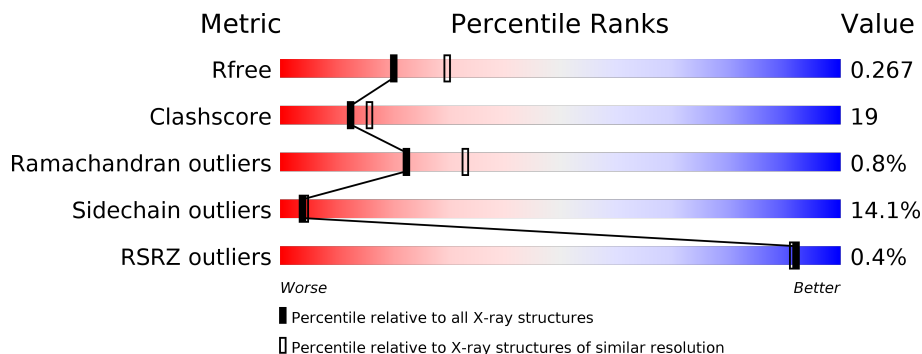
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	135	<div> <div></div> <div>63% 29% 5% .</div> </div>
1	B	135	<div> <div></div> <div>61% 27% 10% .</div> </div>
2	C	125	<div> <div></div> <div>53% 38% 9%</div> </div>
2	D	125	<div> <div></div> <div>51% 33% 13% .</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4515 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 CONVULXIN ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1105	711	182	202	10			
1	B	135	Total	C	N	O	S	0	0	0
			1105	711	182	202	10			

- Molecule 2 is a protein called CONVULXIN BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	0	0
			1054	677	171	196	10			
2	D	125	Total	C	N	O	S	0	0	0
			1054	677	171	196	10			

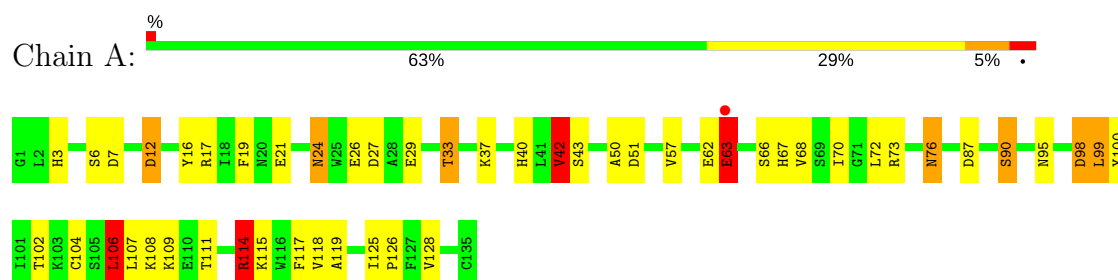
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	57	Total	O	0	0
			57	57		
3	C	43	Total	O	0	0
			43	43		
3	D	48	Total	O	0	0
			48	48		

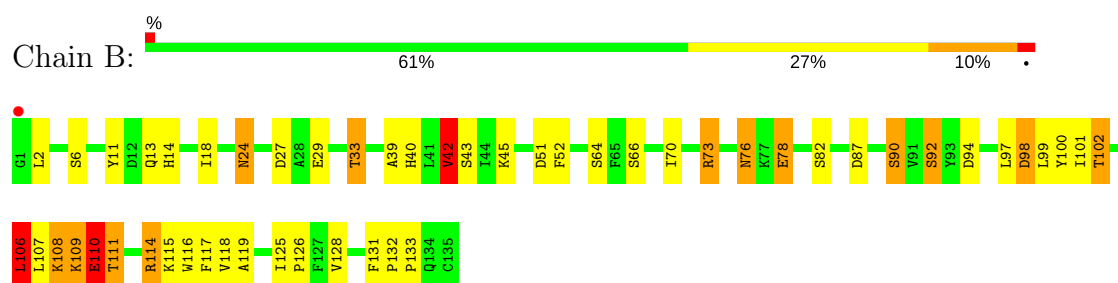
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

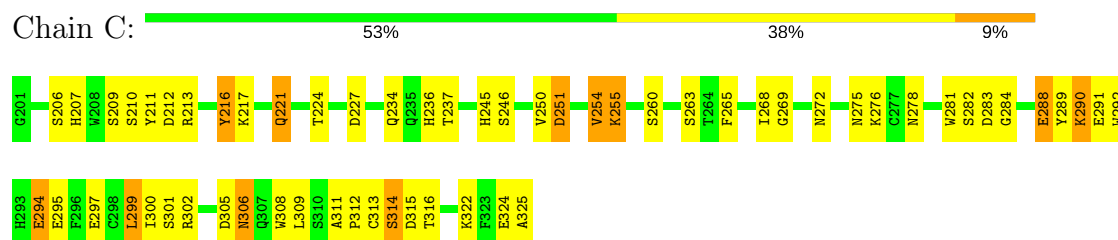
• Molecule 1: CONVULXIN ALPHA



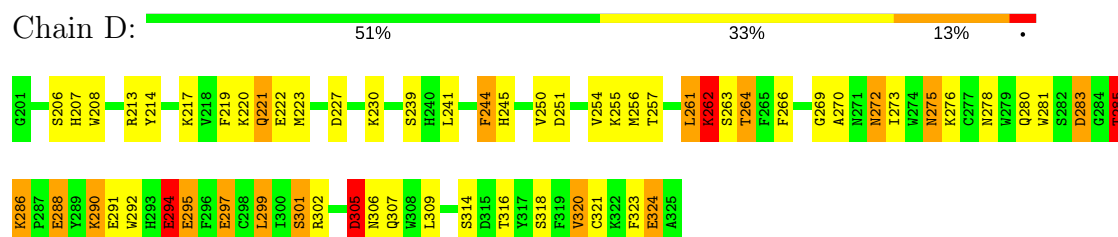
• Molecule 1: CONVULXIN ALPHA



• Molecule 2: CONVULXIN BETA



• Molecule 2: CONVULXIN BETA



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	131.91Å 131.91Å 112.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.40) 97.6 (29.50-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.187 , 0.264 0.196 , 0.267	Depositor DCC
R_{free} test set	1845 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4515	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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

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	A	1.66	10/1138 (0.9%)	1.64	18/1538 (1.2%)
1	B	1.55	8/1138 (0.7%)	1.39	11/1538 (0.7%)
2	C	1.62	12/1094 (1.1%)	1.42	15/1483 (1.0%)
2	D	1.92	17/1094 (1.6%)	1.38	14/1483 (0.9%)
All	All	1.69	47/4464 (1.1%)	1.46	58/6042 (1.0%)

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	A	0	1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CD-OE2	19.65	1.47	1.25
2	D	288	GLU	CD-OE2	17.13	1.44	1.25
2	D	295	GLU	CD-OE2	15.79	1.43	1.25
2	D	294	GLU	CD-OE2	14.16	1.41	1.25
2	D	295	GLU	CD-OE1	12.73	1.39	1.25

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-18.53	111.03	120.30
1	A	114	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	A	63	GLU	OE1-CD-OE2	-14.59	105.79	123.30
1	A	12	ASP	CB-CG-OD2	14.05	130.94	118.30
1	A	73	ARG	NE-CZ-NH1	13.32	126.96	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	GLU	Sidechain

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	1105	0	1053	39	0
1	B	1105	0	1053	44	0
2	C	1054	0	938	31	0
2	D	1054	0	938	60	0
3	A	49	0	0	3	0
3	B	57	0	0	5	0
3	C	43	0	0	1	0
3	D	48	0	0	3	0
All	All	4515	0	3982	155	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 19.

The worst 5 of 155 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:108:LYS:CE	1:B:108:LYS:NZ	1.74	1.46
2:C:221:GLN:H	2:C:221:GLN:HE21	0.97	0.90
2:C:251:ASP:OD1	2:C:306:ASN:ND2	2.04	0.89
2:D:283:ASP:OD2	2:D:285:THR:HB	1.72	0.89
2:D:280:GLN:OE1	2:D:286:LYS:HE3	1.74	0.87

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	A	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	22	33
1	B	133/135 (98%)	123 (92%)	8 (6%)	2 (2%)	12	16
2	C	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	22	33
2	D	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
All	All	512/520 (98%)	473 (92%)	35 (7%)	4 (1%)	22	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	B	110	GLU
2	C	283	ASP
1	B	132	PRO

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	122/122 (100%)	109 (89%)	13 (11%)	8	10
1	B	122/122 (100%)	106 (87%)	16 (13%)	5	5
2	C	116/116 (100%)	98 (84%)	18 (16%)	3	3
2	D	116/116 (100%)	96 (83%)	20 (17%)	2	2
All	All	476/476 (100%)	409 (86%)	67 (14%)	4	4

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	210	SER
2	C	288	GLU
2	D	294	GLU
2	C	221	GLN
2	C	260	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	221	GLN
2	C	245	HIS
2	D	275	ASN
2	C	234	GLN
2	C	236	HIS

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 ⓘ

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	135/135 (100%)	-0.66	1 (0%) 87 86	33, 44, 62, 82	0
1	B	135/135 (100%)	-0.65	1 (0%) 87 86	33, 44, 66, 81	0
2	C	125/125 (100%)	-0.71	0 100 100	33, 44, 65, 78	0
2	D	125/125 (100%)	-0.62	0 100 100	34, 47, 65, 84	0
All	All	520/520 (100%)	-0.66	2 (0%) 92 91	33, 45, 65, 84	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	GLU	2.2
1	B	1	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.