



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:48 pm BST

PDB ID : 5L20
Title : Crystal Structure of a Clostripain (BT_0727) from Bacteroides thetaiotaomicron ATCC 29148 in Complex with Peptide Inhibitor BTN-VLTK-AOMK
Authors : Wolan, D.W.; Roncase, E.J.
Deposited on : 2016-07-29
Resolution : 1.45 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 : 2.11
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) : 2.11

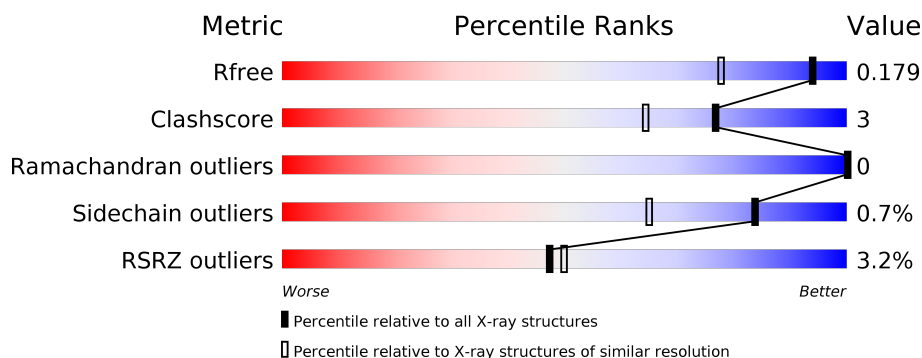
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 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	143	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	229	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>
3	C	5	<div> <div>60%</div> <div>40%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3173 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 Clostripain-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	5	0
			932	594	148	183	7			

- Molecule 2 is a protein called Clostripain-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	3	0
			1764	1131	270	352	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	394	LEU	-	expression tag	UNP Q8A9T8
B	395	GLU	-	expression tag	UNP Q8A9T8
B	396	HIS	-	expression tag	UNP Q8A9T8
B	397	HIS	-	expression tag	UNP Q8A9T8
B	398	HIS	-	expression tag	UNP Q8A9T8
B	399	HIS	-	expression tag	UNP Q8A9T8
B	400	HIS	-	expression tag	UNP Q8A9T8
B	401	HIS	-	expression tag	UNP Q8A9T8

- Molecule 3 is a protein called Peptide Inhibitor BTN-VLTK-AOMK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			36	25	5	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		

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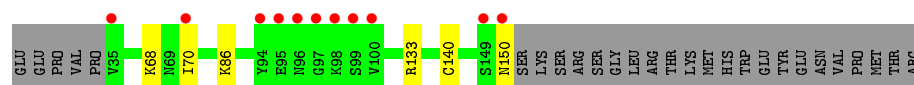
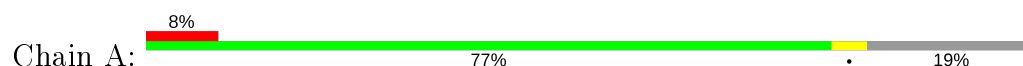
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	316	Total 316	O 316	0	0
4	C	3	Total 3	O 3	0	0

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 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: Clostripain-related protein



- Molecule 2: Clostripain-related protein



- Molecule 3: Peptide Inhibitor BTN-VLTK-AOMK



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.21 Å 102.89 Å 84.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 1.45 43.90 – 1.45	Depositor EDS
% Data completeness (in resolution range)	89.0 (43.90-1.45) 89.0 (43.90-1.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.45 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.150 , 0.179 0.151 , 0.179	Depositor DCC
R_{free} test set	2729 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3173	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: BTN, CKC

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	0.49	0/965	0.67	1/1316 (0.1%)
2	B	0.56	0/1816	0.69	1/2468 (0.0%)
3	C	0.46	0/21	0.66	0/28
All	All	0.53	0/2802	0.68	2/3812 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	356	MET	CG-SD-CE	10.82	117.51	100.20
1	A	133	ARG	NE-CZ-NH1	6.91	123.76	120.30

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	932	0	905	3	0
2	B	1764	0	1677	13	0
3	C	36	0	41	4	0
4	A	122	0	0	1	2
4	B	316	0	0	5	2
4	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3173	0	2623	16	2

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 3.

All (16) 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)
2:B:356:MET:HE3	3:C:404:THR:H	1.30	0.95
2:B:356:MET:CE	3:C:404:THR:H	1.92	0.82
2:B:283:ASN:ND2	4:B:502:HOH:O	2.17	0.76
2:B:290:GLU:OE1	4:B:501:HOH:O	2.17	0.57
1:A:68:LYS:HB2	1:A:70:ILE:HD11	1.86	0.57
2:B:178:ASN:HB3	4:B:661:HOH:O	2.06	0.56
2:B:356:MET:HE3	3:C:404:THR:N	2.11	0.54
2:B:294:ARG:NH2	2:B:329:ASP:OD2	2.49	0.46
2:B:206:ASP:CG	4:B:508:HOH:O	2.57	0.43
1:A:86:LYS:HB3	1:A:86:LYS:HE2	1.83	0.42
2:B:207:CYS:SG	2:B:231:GLU:HA	2.60	0.42
2:B:356:MET:HE2	3:C:403:LEU:HA	2.01	0.41
2:B:263:TYR:O	2:B:269:PRO:HA	2.20	0.41
1:A:150:ASN:HB3	4:A:594:HOH:O	2.21	0.41
2:B:193[B]:SER:OG	4:B:503:HOH:O	2.21	0.41
2:B:237:MET:HB2	2:B:239:TYR:CZ	2.55	0.41

All (2) 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)
4:A:504:HOH:O	4:B:697:HOH:O[4_555]	2.01	0.19
4:A:538:HOH:O	4:B:753:HOH:O[6_555]	2.17	0.03

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	119/143 (83%)	113 (95%)	6 (5%)	0	100	100
2	B	224/229 (98%)	222 (99%)	2 (1%)	0	100	100
3	C	1/5 (20%)	1 (100%)	0	0	100	100
All	All	344/377 (91%)	336 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	107/132 (81%)	105 (98%)	2 (2%)	57	23
2	B	193/199 (97%)	192 (100%)	1 (0%)	88	75
3	C	3/3 (100%)	3 (100%)	0	100	100
All	All	303/334 (91%)	300 (99%)	3 (1%)	84	52

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140[A]	CYS
1	A	140[B]	CYS
2	B	211	SER

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

5.3.3 RNA ⓘ

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, 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	116/143 (81%)	0.09	11 (9%) 8 9	10, 16, 43, 68	0
2	B	223/229 (97%)	-0.26	0 100 100	9, 13, 27, 35	0
3	C	3/5 (60%)	-0.14	0 100 100	16, 16, 20, 22	0
All	All	342/377 (90%)	-0.14	11 (3%) 47 50	9, 15, 31, 68	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ASN	5.9
1	A	70	ILE	4.8
1	A	150	ASN	4.4
1	A	97	GLY	4.3
1	A	100	VAL	3.9
1	A	35	VAL	3.8
1	A	149	SER	3.5
1	A	94	TYR	3.2
1	A	98	LYS	2.9
1	A	95	GLU	2.0
1	A	99	SER	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.