wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:00 AM GMT

PDB ID	:	2F2F
Title	:	Crystal structure of cytolethal distending toxin (CDT) from Actinobacillus a ctinomycetemcomitans
Authors	:	Yamada, T.; Komoto, J.; Saiki, K.; Konishi, K.; Takusagawa, F.
Deposited on	:	2005-11-16
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

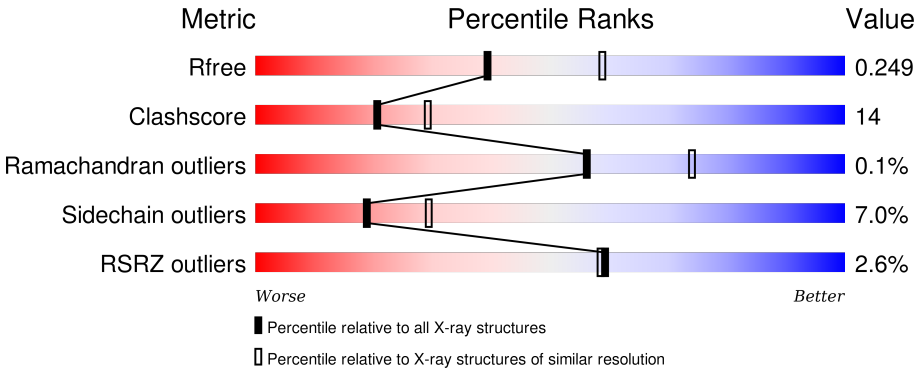
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 <=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	222	55% 14% 31%
1	D	222	57% 12% 31%
2	B	283	68% 20% 8%
2	E	283	66% 23% 8%
3	C	186	6% 56% 22% 17%

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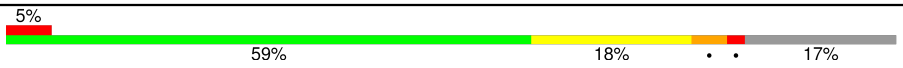
Mol	Chain	Length	Quality of chain
3	F	186	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9188 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 Cytolethal distending toxin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1207	770	201	230	6			
1	D	153	Total	C	N	O	S	0	0	0
			1207	770	201	230	6			

- Molecule 2 is a protein called Cytolethal distending toxin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			2038	1268	378	388	4			
2	E	261	Total	C	N	O	S	0	0	0
			2038	1268	378	388	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	HIS	ARG	see remark 999	UNP Q7DK12
E	281	HIS	ARG	see remark 999	UNP Q7DK12

- Molecule 3 is a protein called cytolethal distending toxin C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	154	Total	C	N	O	S	0	0	0
			1213	781	200	227	5			
3	F	154	Total	C	N	O	S	0	0	0
			1213	781	200	227	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	172	PRO	SER	see remark 999	UNP Q7DK11
F	172	PRO	SER	see remark 999	UNP Q7DK11

- Molecule 4 is water.

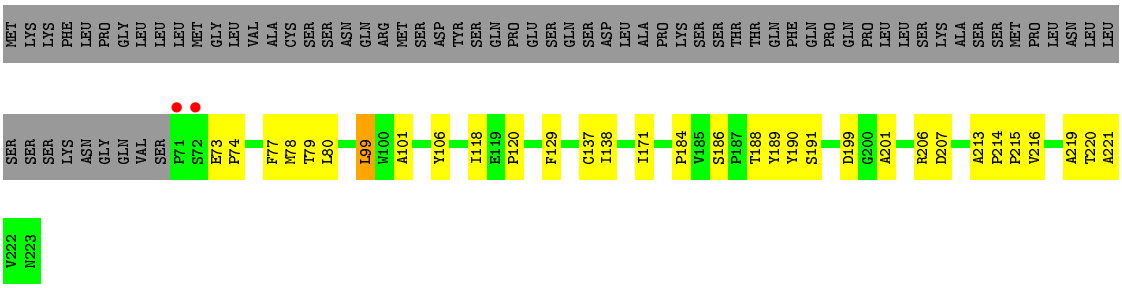
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	60	Total O 60 60	0	0
4	C	32	Total O 32 32	0	0
4	D	41	Total O 41 41	0	0
4	E	64	Total O 64 64	0	0
4	F	38	Total O 38 38	0	0

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 errors 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.

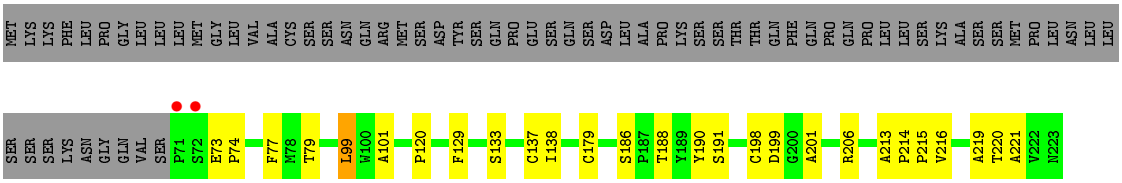
- Molecule 1: Cytolethal distending toxin A

Chain A:



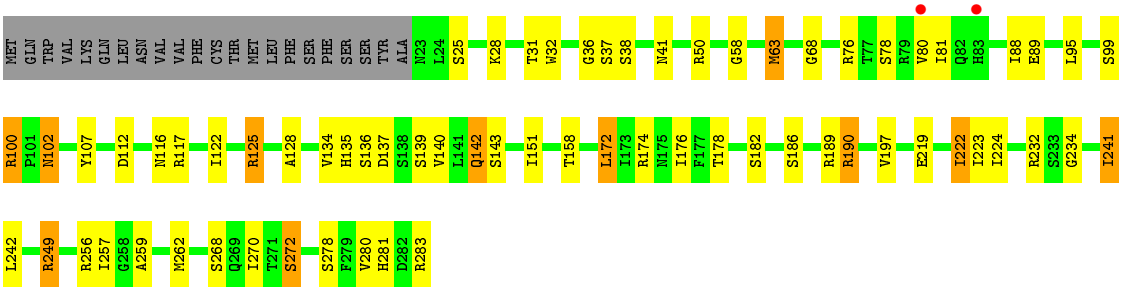
- Molecule 1: Cytolethal distending toxin A

Chain D:



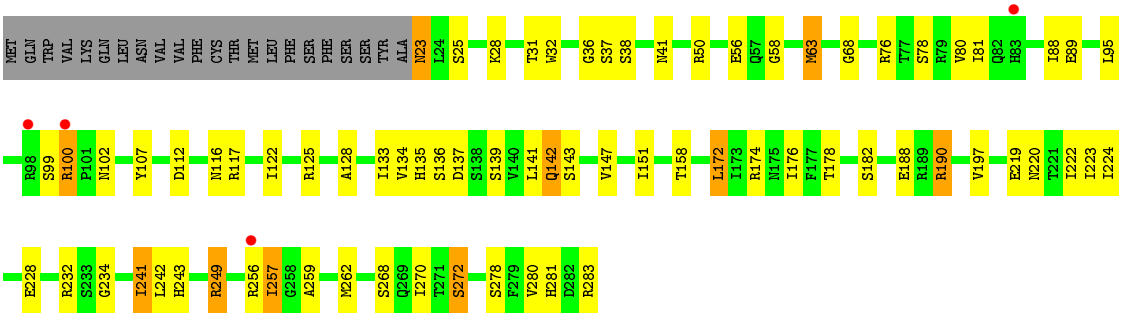
- Molecule 2: Cytolethal distending toxin B

Chain B:

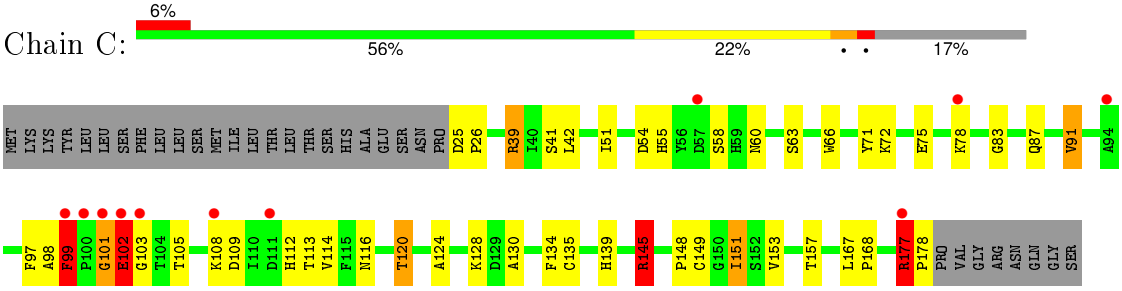


- Molecule 2: Cytolethal distending toxin B

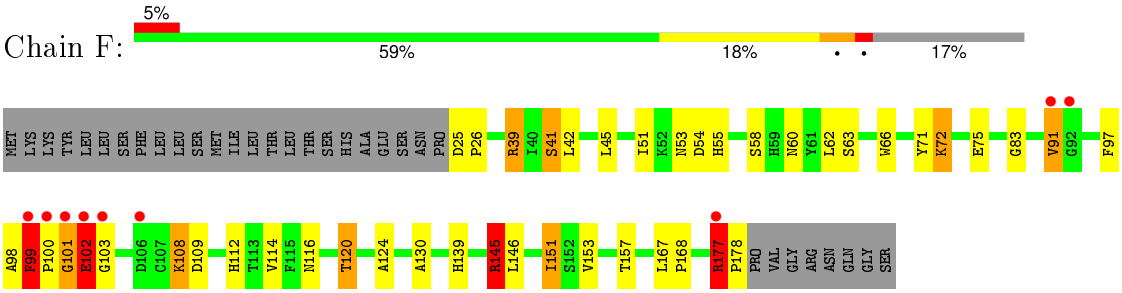
Chain E:



- Molecule 3: cytolethal distending toxin C



- Molecule 3: cytolethal distending toxin C



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.65Å 117.46Å 123.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 48.20 – 2.38	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 99.5 (48.20-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.31 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.251 0.216 , 0.249	Depositor DCC
R_{free} test set	6689 reflections (10.11%)	DCC
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	1.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	12 of 67573 reflections (0.018%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9188	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.12 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.8088e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/1241	0.71	0/1696
1	D	0.48	0/1241	0.72	0/1696
2	B	0.45	0/2080	0.77	2/2828 (0.1%)
2	E	0.45	0/2080	0.78	2/2828 (0.1%)
3	C	0.53	0/1249	0.90	7/1701 (0.4%)
3	F	0.53	0/1249	0.88	9/1701 (0.5%)
All	All	0.48	0/9140	0.79	20/12450 (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
2	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	99	PHE	C-N-CD	10.54	150.53	128.40
3	F	99	PHE	C-N-CD	-9.58	99.51	120.60
3	C	177	ARG	NE-CZ-NH1	8.76	124.68	120.30
2	B	190	ARG	NE-CZ-NH2	-7.46	116.57	120.30
3	F	99	PHE	N-CA-C	-7.39	91.06	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	107	TYR	Sidechain
2	E	107	TYR	Sidechain

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	1207	0	1164	34	0
1	D	1207	0	1164	23	0
2	B	2038	0	2003	55	0
2	E	2038	0	2003	57	0
3	C	1213	0	1185	48	0
3	F	1213	0	1185	54	0
4	A	37	0	0	0	0
4	B	60	0	0	1	0
4	C	32	0	0	0	0
4	D	41	0	0	0	0
4	E	64	0	0	4	0
4	F	38	0	0	1	0
All	All	9188	0	8704	249	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 14.

The worst 5 of 249 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:F:177:ARG:HA	3:F:177:ARG:HE	1.11	1.08
3:F:177:ARG:HA	3:F:177:ARG:NE	1.83	0.94
3:F:25:ASP:HB3	3:F:26:PRO:CD	1.98	0.93
2:E:135:HIS:HD2	2:E:139:SER:HB2	1.34	0.92
3:C:25:ASP:HB3	3:C:26:PRO:CD	2.01	0.90

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	151/222 (68%)	145 (96%)	6 (4%)	0	100 100
1	D	151/222 (68%)	145 (96%)	6 (4%)	0	100 100
2	B	259/283 (92%)	248 (96%)	11 (4%)	0	100 100
2	E	259/283 (92%)	247 (95%)	12 (5%)	0	100 100
3	C	152/186 (82%)	147 (97%)	4 (3%)	1 (1%)	26 38
3	F	152/186 (82%)	147 (97%)	5 (3%)	0	100 100
All	All	1124/1382 (81%)	1079 (96%)	44 (4%)	1 (0%)	56 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	101	GLY

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	132/195 (68%)	130 (98%)	2 (2%)	72 87
1	D	132/195 (68%)	129 (98%)	3 (2%)	58 78
2	B	223/244 (91%)	206 (92%)	17 (8%)	16 25
2	E	223/244 (91%)	203 (91%)	20 (9%)	12 17
3	C	135/164 (82%)	121 (90%)	14 (10%)	9 12
3	F	135/164 (82%)	122 (90%)	13 (10%)	10 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	980/1206 (81%)	911 (93%)	69 (7%)	19 29

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	151	ILE
2	E	63	MET
3	F	102	GLU
3	C	177	ARG
1	D	216	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	55	HIS
3	C	112	HIS
2	E	135	HIS
2	B	281	HIS
2	E	102	ASN

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

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

6.1 Protein, DNA and RNA chains

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^{th} 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	153/222 (68%)	-0.28	2 (1%)	79 79	2, 8, 23, 51	0
1	D	153/222 (68%)	-0.24	2 (1%)	79 79	2, 8, 23, 47	0
2	B	261/283 (92%)	-0.29	2 (0%)	87 87	2, 6, 25, 44	0
2	E	261/283 (92%)	-0.22	4 (1%)	76 75	2, 7, 26, 44	0
3	C	154/186 (82%)	0.18	11 (7%)	19 19	3, 15, 39, 65	0
3	F	154/186 (82%)	0.04	9 (5%)	26 27	3, 11, 33, 50	0
All	All	1136/1382 (82%)	-0.16	30 (2%)	59 58	2, 8, 29, 65	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	PRO	9.3
1	D	71	PRO	9.1
3	F	100	PRO	7.8
1	D	72	SER	7.8
3	C	101	GLY	7.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.