Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 07:23 pm BST

PDB ID	:	5T87
Title	:	Crystal structure of CDI complex from Cupriavidus taiwanensis LMG 19424
Authors	:	Michalska, K.; Joachimiak, G.; Jedrzejczak, R.; Hayes, C.S.; Goulding, C.W.; Joachimiak, A.; Structure-Function Analysis of Polymorphic CDI Toxin-Immunity Protein Complexes (UC4CDI); Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2016-09-06
Resolution	:	2.40 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 (i) symbol.

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

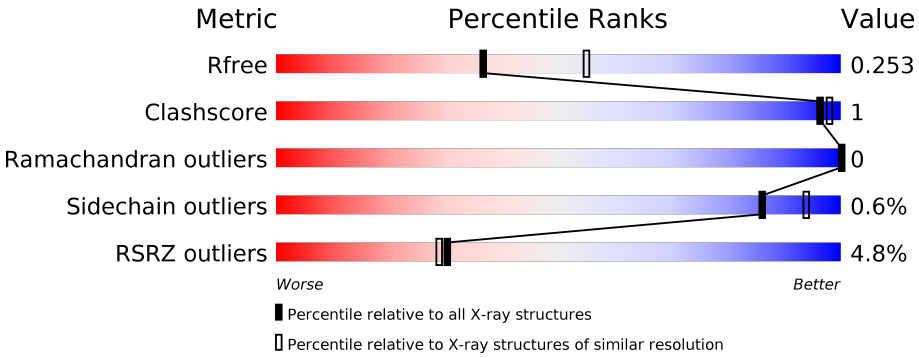
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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 <=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	116	2% 98%
1	B	116	93%
1	C	116	3% 92% 6%
1	D	116	3% 97%
2	E	76	17% 86% 5% 9%
2	F	76	5% 97%

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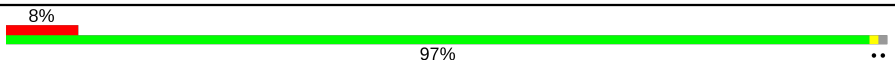
Mol	Chain	Length	Quality of chain
2	G	76	
2	H	76	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6002 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 CdiI immunity protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	Se	0	1	0
			899	562	160	172	2	3			
1	B	113	Total	C	N	O	S	Se	0	1	0
			888	556	156	171	2	3			
1	C	115	Total	C	N	O	S	Se	0	1	0
			904	565	158	175	2	4			
1	D	115	Total	C	N	O	S	Se	0	2	0
			915	571	161	178	2	3			

- Molecule 2 is a protein called CdiA toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	69	Total	C	N	O	Se	0	0	0
			539	331	101	106	1			
2	F	74	Total	C	N	O	Se	0	0	0
			578	354	111	112	1			
2	G	75	Total	C	N	O	Se	0	0	0
			587	360	113	113	1			
2	H	70	Total	C	N	O	Se	0	0	0
			548	337	103	107	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	36	Total	O	0	0
			36	36		
3	C	35	Total	O	0	0
			35	35		
3	D	31	Total	O	0	0
			31	31		

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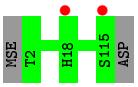
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	3	Total O 3 3	0	0
3	F	10	Total O 10 10	0	0
3	G	9	Total O 9 9	0	0
3	H	6	Total O 6 6	0	0

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.

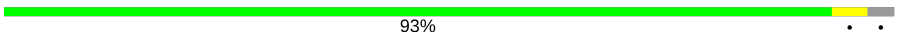
- Molecule 1: CdiI immunity protein

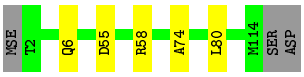
Chain A:



- Molecule 1: CdiI immunity protein

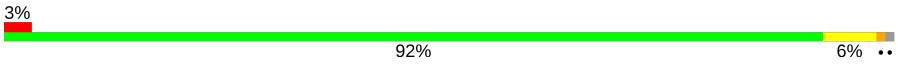
Chain B:

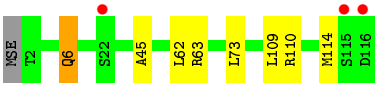




- Molecule 1: CdiI immunity protein

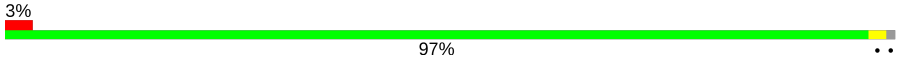
Chain C:

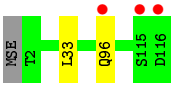




- Molecule 1: CdiI immunity protein

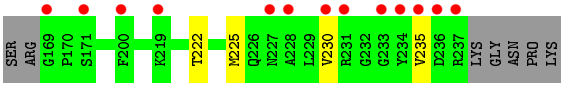
Chain D:





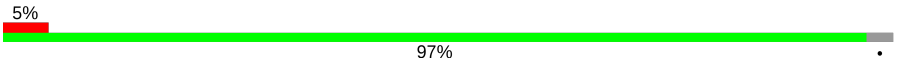
- Molecule 2: CdiA toxin

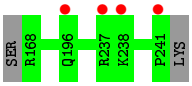
Chain E:



- Molecule 2: CdiA toxin

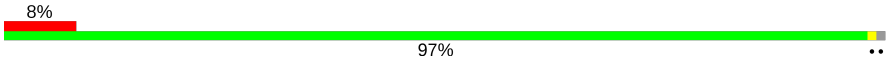
Chain F:

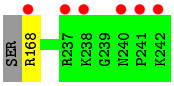




- Molecule 2: CdiA toxin

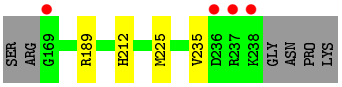
Chain G:





- Molecule 2: CdiA toxin

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.10Å 107.10Å 315.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.40) 98.8 (30.03-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.215 , 0.247 0.218 , 0.253	Depositor DCC
R_{free} test set	1090 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 23.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6002	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.50	0/913	0.70	0/1233
1	B	0.51	0/902	0.72	0/1219
1	C	0.52	0/918	0.77	1/1240 (0.1%)
1	D	0.51	0/930	0.71	0/1257
2	E	0.50	0/548	0.62	0/741
2	F	0.54	0/588	0.70	0/794
2	G	0.53	0/597	0.74	0/805
2	H	0.50	0/557	0.68	0/752
All	All	0.51	0/5953	0.71	1/8041 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	ARG	NE-CZ-NH2	-5.89	117.36	120.30

There are no chirality outliers.

There are no planarity outliers.

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	899	0	871	0	0
1	B	888	0	858	2	1
1	C	904	0	871	5	1
1	D	915	0	874	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	539	0	517	2	0
2	F	578	0	559	0	0
2	G	587	0	572	0	0
2	H	548	0	530	2	0
3	A	14	0	0	0	0
3	B	36	0	0	0	0
3	C	35	0	0	0	0
3	D	31	0	0	0	0
3	E	3	0	0	0	0
3	F	10	0	0	0	0
3	G	9	0	0	0	0
3	H	6	0	0	0	0
All	All	6002	0	5652	11	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 1.

All (11) 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:E:230:VAL:HG22	2:E:235:VAL:HG13	1.87	0.55
1:C:110:ARG:HG3	1:C:114:MSE:HE3	1.93	0.50
1:B:55:ASP:HB3	1:B:58:ARG:HG3	1.94	0.49
2:E:222:THR:HG23	2:E:225:MSE:HE3	1.95	0.48
1:D:33:LEU:HD21	2:H:212:HIS:CE1	2.50	0.46
1:C:109:LEU:HD23	1:C:114:MSE:HE2	2.00	0.44
1:C:45:ALA:HB3	1:C:73:LEU:HD21	2.00	0.43
2:H:189:ARG:HD3	2:H:225:MSE:HE2	2.00	0.43
1:C:109:LEU:HG	1:C:114:MSE:HE2	2.02	0.42
1:B:74:ALA:HA	1:B:80:LEU:HD13	2.00	0.42
1:C:109:LEU:CG	1:C:114:MSE:HE2	2.51	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)
1:D:96:GLN:OE1	1:D:96:GLN:OE1[12_565]	1.90	0.30
1:B:6:GLN:OE1	1:C:6:GLN:NE2[7_565]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
1	B	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
1	C	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
1	D	115/116 (99%)	115 (100%)	0	0	100	100
2	E	67/76 (88%)	60 (90%)	7 (10%)	0	100	100
2	F	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
2	G	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
2	H	68/76 (90%)	66 (97%)	2 (3%)	0	100	100
All	All	734/768 (96%)	714 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	93/90 (103%)	93 (100%)	0	100	100
1	B	92/90 (102%)	92 (100%)	0	100	100
1	C	94/90 (104%)	92 (98%)	2 (2%)	53	72
1	D	95/90 (106%)	95 (100%)	0	100	100
2	E	60/65 (92%)	60 (100%)	0	100	100
2	F	64/65 (98%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	65/65 (100%)	64 (98%)	1 (2%)	65 80
2	H	61/65 (94%)	60 (98%)	1 (2%)	62 79
All	All	624/620 (101%)	620 (99%)	4 (1%)	86 94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	GLN
1	C	62	LEU
2	G	168	ARG
2	H	235	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	172	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	111/116 (95%)	-0.21	2 (1%) 68 66	38, 52, 68, 89	0
1	B	110/116 (94%)	-0.38	0 100 100	34, 42, 55, 59	0
1	C	112/116 (96%)	-0.30	3 (2%) 54 52	33, 41, 55, 99	0
1	D	112/116 (96%)	-0.09	3 (2%) 54 52	33, 44, 60, 99	0
2	E	68/76 (89%)	0.94	13 (19%) 1 0	43, 83, 116, 130	0
2	F	73/76 (96%)	-0.03	4 (5%) 25 24	37, 50, 84, 95	0
2	G	74/76 (97%)	0.08	6 (8%) 12 11	38, 52, 102, 111	0
2	H	69/76 (90%)	-0.03	4 (5%) 23 22	39, 56, 86, 113	0
All	All	729/768 (94%)	-0.06	35 (4%) 30 29	33, 47, 94, 130	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	116	ASP	6.9
2	E	234	TYR	5.5
2	E	169	GLY	4.9
2	E	236	ASP	4.6
1	C	116	ASP	4.4
2	E	171	SER	4.4
2	E	230	VAL	4.0
2	H	237	ARG	4.0
2	G	242	LYS	3.8
2	H	236	ASP	3.8
1	D	115	SER	3.5
1	A	115	SER	3.4
2	E	231	ARG	3.4
2	G	241	PRO	3.1
2	E	237	ARG	2.9
2	F	196	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	G	238	LYS	2.9
2	F	238	LYS	2.9
1	D	96	GLN	2.8
2	E	219	LYS	2.8
2	E	228	ALA	2.7
2	F	237	ARG	2.6
2	H	238	LYS	2.6
2	E	233	GLY	2.5
2	H	169	GLY	2.5
2	E	235	VAL	2.4
2	E	227	ASN	2.4
1	A	18	HIS	2.3
2	G	237	ARG	2.3
2	G	168	ARG	2.2
2	E	200	PHE	2.2
2	G	240	ASN	2.2
1	C	22	SER	2.1
1	C	115	SER	2.1
2	F	241	PRO	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 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.