



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 02:17 PM JST

PDB ID : 7FIW
Title : Crystal structure of the complex formed by Wolbachia cytoplasmic incompatibility factors CidAwMel(ST) and CidBND1-ND2 from wPip(Pel)
Authors : Xiao, Y.J.; Wang, W.; Chen, X.; Ji, X.Y.; Yang, H.T.
Deposited on : 2021-08-01
Resolution : 2.16 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
Xtriage (Phenix)	:	1.13
EDS	:	2.27
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)	:	2.27

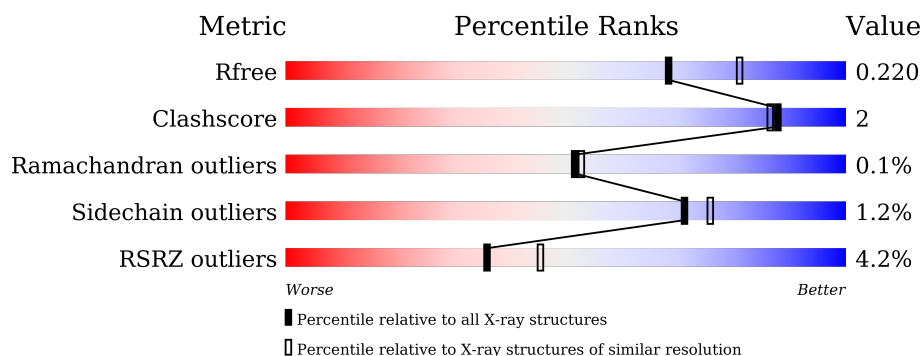
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 of 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	769	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>
2	B	482	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>.</div> <div>15%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10076 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 ULP_PROTEASE domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	14	0
			6045	3782	1119	1129	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	LEU	-	expression tag	UNP B3CP63
A	763	GLU	-	expression tag	UNP B3CP63
A	764	HIS	-	expression tag	UNP B3CP63
A	765	HIS	-	expression tag	UNP B3CP63
A	766	HIS	-	expression tag	UNP B3CP63
A	767	HIS	-	expression tag	UNP B3CP63
A	768	HIS	-	expression tag	UNP B3CP63
A	769	HIS	-	expression tag	UNP B3CP63

- Molecule 2 is a protein called bacteria factor 4,CidA I(Zeta/1) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	411	Total	C	N	O	S	0	0	0
			3388	2177	570	625	16			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	LYS	ARG	engineered mutation	UNP Q73HD5
B	47	TYR	LEU	engineered mutation	UNP Q73HD5
B	93	ARG	PRO	engineered mutation	UNP Q73HD5
B	288	ARG	GLN	engineered mutation	UNP Q73HD5
B	295	SER	TYR	engineered mutation	UNP Q73HD5
B	299	ASP	ASN	engineered mutation	UNP Q73HD5
B	347	GLU	GLY	engineered mutation	UNP Q73HD5
B	393	ARG	GLU	engineered mutation	UNP Q73HD5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	397	LEU	ILE	engineered mutation	UNP Q73HD5
B	475	LEU	-	expression tag	UNP Q73HD5
B	476	GLU	-	expression tag	UNP Q73HD5
B	477	HIS	-	expression tag	UNP Q73HD5
B	478	HIS	-	expression tag	UNP Q73HD5
B	479	HIS	-	expression tag	UNP Q73HD5
B	480	HIS	-	expression tag	UNP Q73HD5
B	481	HIS	-	expression tag	UNP Q73HD5
B	482	HIS	-	expression tag	UNP Q73HD5

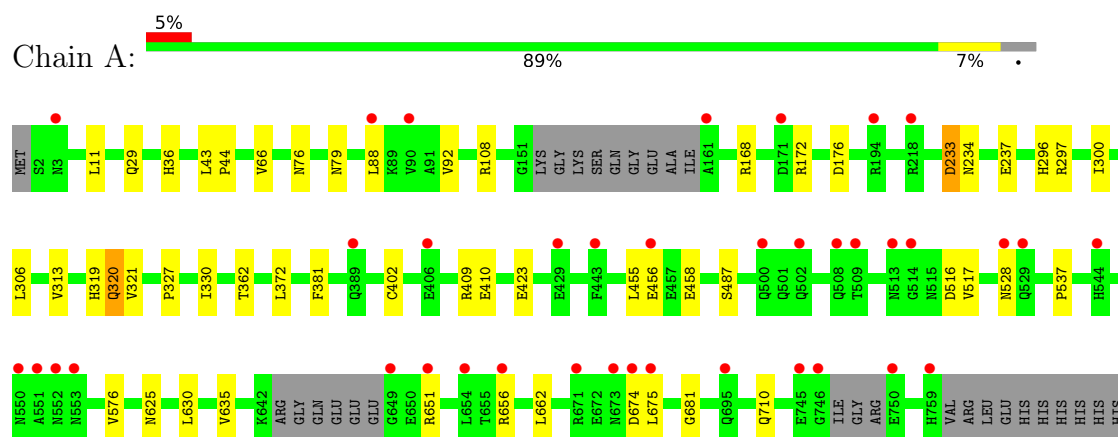
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	383	Total O 383 383	0	0
3	B	260	Total O 260 260	0	0

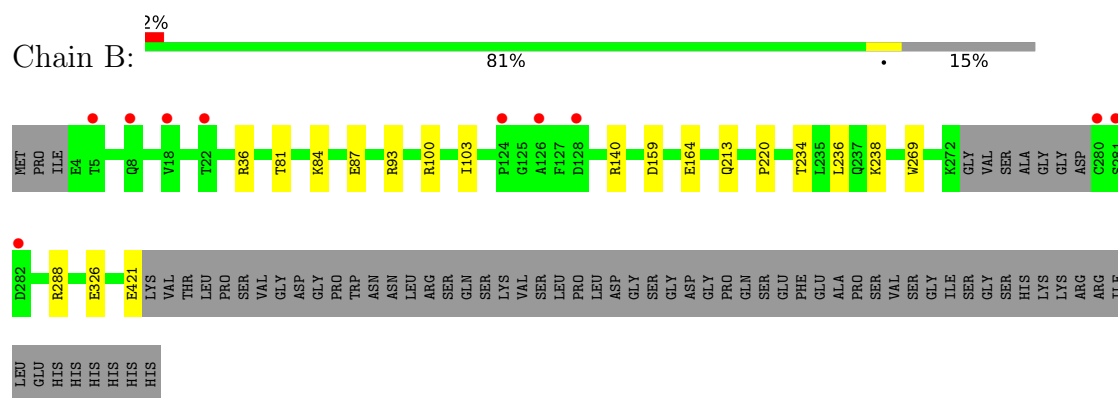
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ULP_PROTEASE domain-containing protein



- Molecule 2: bacteria factor 4,CidA I(Zeta/1) protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.36Å 98.69Å 184.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.62 – 2.16 31.62 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.4 (31.62-2.16) 98.4 (31.62-2.16)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.192 , 0.220 0.192 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10076	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.26	0/6209	0.51	0/8407
2	B	0.25	0/3456	0.46	0/4641
All	All	0.25	0/9665	0.49	0/13048

There are no bond length outliers.

There are no bond angle outliers.

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	6045	0	5817	28	0
2	B	3388	0	3391	12	0
3	A	383	0	0	2	0
3	B	260	0	0	1	0
All	All	10076	0	9208	37	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 2.

All (37) 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:A:66:VAL:HG22	1:A:92:VAL:HG22	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:GLU:H	2:B:326:GLU:CD	2.14	0.51
1:A:409:ARG:HD3	1:A:537:PRO:HD3	1.91	0.51
1:A:320:GLN:HG3	1:A:321:VAL:HG13	1.93	0.51
1:A:635:VAL:HG12	1:A:710[B]:GLN:HG2	1.92	0.51
2:B:84:LYS:HE2	2:B:87:GLU:HA	1.92	0.51
1:A:516:ASP:N	1:A:516:ASP:OD1	2.43	0.51
1:A:576:VAL:HG21	1:A:625:ASN:HB3	1.93	0.51
1:A:237:GLU:OE1	1:A:319:HIS:NE2	2.47	0.48
1:A:297:ARG:NH2	3:A:815:HOH:O	2.46	0.47
1:A:29[A]:GLN:HB3	1:A:300:ILE:O	2.15	0.46
2:B:159:ASP:HB3	2:B:164:GLU:HG2	1.96	0.46
2:B:213:GLN:HB3	3:B:581:HOH:O	2.16	0.46
1:A:313:VAL:HG13	1:A:330:ILE:HB	1.98	0.45
2:B:81:THR:HG21	2:B:103:ILE:HG13	1.99	0.45
1:A:36:HIS:CE1	1:A:306:LEU:HB2	2.52	0.45
1:A:172:ARG:HD3	1:A:176:ASP:O	2.16	0.45
1:A:662:LEU:HD21	1:A:681:GLY:HA3	1.97	0.44
1:A:458:GLU:HG2	2:B:93:ARG:HA	1.99	0.44
1:A:233:ASP:OD1	1:A:233:ASP:N	2.51	0.43
1:A:327:PRO:HG3	1:A:362:THR:HG21	2.00	0.43
1:A:455:LEU:O	2:B:93:ARG:NH1	2.51	0.43
2:B:288:ARG:HD2	2:B:288:ARG:HA	1.86	0.43
2:B:236:LEU:HB2	2:B:269:TRP:CE2	2.54	0.42
1:A:44:PRO:HB3	1:A:88:LEU:HB2	2.01	0.42
1:A:168:ARG:NH2	1:A:651:ARG:HH21	2.18	0.42
1:A:372:LEU:HD13	1:A:381:PHE:HB3	2.01	0.42
1:A:410:GLU:OE1	1:A:410:GLU:N	2.53	0.41
1:A:234:ASN:ND2	3:A:815:HOH:O	2.53	0.41
1:A:487:SER:O	1:A:517:VAL:HG13	2.20	0.41
1:A:43:LEU:HB3	1:A:44:PRO:HD3	2.02	0.41
1:A:76:ASN:HB3	1:A:79:ASN:OD1	2.21	0.41
2:B:234:THR:O	2:B:238:LYS:HG2	2.22	0.40
1:A:296:HIS:CD2	1:A:297:ARG:HG3	2.56	0.40
1:A:456:GLU:O	2:B:93:ARG:NH1	2.54	0.40
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.93	0.40
2:B:36:ARG:HD2	2:B:220:PRO:HG3	2.04	0.40

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	746/769 (97%)	734 (98%)	11 (2%)	1 (0%)	51	53
2	B	407/482 (84%)	401 (98%)	6 (2%)	0	100	100
All	All	1153/1251 (92%)	1135 (98%)	17 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLN

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	655/680 (96%)	646 (99%)	9 (1%)	67	72
2	B	369/433 (85%)	366 (99%)	3 (1%)	81	86
All	All	1024/1113 (92%)	1012 (99%)	12 (1%)	71	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	233	ASP
1	A	402	CYS
1	A	423	GLU
1	A	528	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	630	LEU
1	A	656	ARG
1	A	674	ASP
1	A	675	LEU
2	B	100	ARG
2	B	140	ARG
2	B	421	GLU

Sometimes 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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, 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	740/769 (96%)	0.20	38 (5%) 28 36	26, 48, 75, 97	0
2	B	411/482 (85%)	0.08	10 (2%) 59 67	31, 49, 75, 105	0
All	All	1151/1251 (92%)	0.16	48 (4%) 36 45	26, 48, 75, 105	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	ALA	6.6
2	B	5	THR	6.5
2	B	280	CYS	5.6
2	B	124	PRO	4.3
1	A	759	HIS	4.1
2	B	282	ASP	3.6
2	B	281	SER	3.5
1	A	651	ARG	3.4
2	B	128	ASP	3.3
1	A	671	ARG	3.1
1	A	513	ASN	3.1
2	B	8	GLN	3.0
1	A	746	GLY	3.0
1	A	528	ASN	2.9
1	A	3	ASN	2.8
1	A	90	VAL	2.8
1	A	674	ASP	2.7
1	A	551	ALA	2.7
1	A	171	ASP	2.7
1	A	502	GLN	2.6
1	A	553	ASN	2.6
1	A	514	GLY	2.6
2	B	126	ALA	2.6
1	A	406	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	656	ARG	2.5
1	A	529[A]	GLN	2.5
1	A	649	GLY	2.4
1	A	750	GLU	2.4
1	A	389	GLN	2.3
1	A	429	GLU	2.3
1	A	509	THR	2.3
1	A	544	HIS	2.3
1	A	218	ARG	2.2
1	A	552	ASN	2.2
1	A	194	ARG	2.2
1	A	508	GLN	2.2
1	A	695	GLN	2.2
1	A	673	ASN	2.2
1	A	456	GLU	2.2
1	A	654	LEU	2.1
1	A	500	GLN	2.1
1	A	88	LEU	2.1
2	B	18	VAL	2.1
2	B	22	THR	2.1
1	A	443	PHE	2.0
1	A	675	LEU	2.0
1	A	745	GLU	2.0
1	A	550[A]	ASN	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 monosaccharides 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.