Full wwPDB X-ray Structure Validation Report (i)

May 4, 2024 – 06:12 pm BST

PDB ID	:	6HUI
Title	:	The structure of Dps from Listeria innocua soaked with zinc
Authors	:	Zeth, K.; Okuda, M.
Deposited on	:	2018-10-08
Resolution	:	3.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

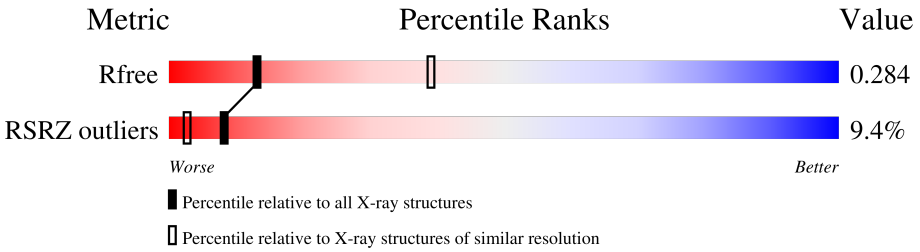
MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	2092 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	214	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7398 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 DNA protection during starvation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1222	784	196	235	7	0	0	0
1	B	150	1222	784	196	235	7	0	0	0
1	C	149	1215	779	195	234	7	0	0	0
1	D	150	1222	784	196	235	7	0	0	0
1	E	152	1236	791	199	239	7	0	0	0
1	F	150	1219	782	196	234	7	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	17	17	17	0	0
2	B	16	16	16	0	0
2	C	8	8	8	0	0
2	D	12	12	12	0	0
2	E	3	3	3	0	0
2	F	6	6	6	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.33Å 86.33Å 269.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.70 – 3.00 45.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.70-3.00) 99.6 (45.70-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.228 , 0.284 0.228 , 0.284	Depositor DCC
R_{free} test set	1066 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	109.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 84.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7398	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 62 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 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	150/156 (96%)	0.19	8 (5%)	26	10	102, 134, 177, 239	0
1	B	150/156 (96%)	0.65	17 (11%)	5	1	109, 154, 217, 248	0
1	C	149/156 (95%)	0.46	10 (6%)	17	5	96, 132, 175, 204	0
1	D	150/156 (96%)	0.30	6 (4%)	38	15	87, 123, 164, 217	0
1	E	152/156 (97%)	0.46	16 (10%)	6	2	101, 143, 190, 239	0
1	F	150/156 (96%)	0.98	28 (18%)	1	0	132, 173, 215, 270	0
All	All	901/936 (96%)	0.51	85 (9%)	8	3	87, 143, 199, 270	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	114	TYR	6.7
1	F	96	MET	5.6
1	B	144	ILE	5.3
1	A	125	GLY	5.3
1	F	35	MET	4.6
1	C	114	TYR	4.2
1	B	137	LYS	4.0
1	F	23	VAL	3.8
1	F	133	LEU	3.8
1	E	114	TYR	3.6
1	E	20	ASN	3.6
1	F	36	ARG	3.5
1	B	35	MET	3.5
1	E	39	ASN	3.5
1	A	68	ILE	3.5
1	E	7	SER	3.4
1	F	157	GLU	3.3
1	E	157	GLU	3.2
1	F	65	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	114	TYR	3.2
1	B	13	PHE	3.1
1	F	150	PHE	3.1
1	F	100	MET	3.1
1	F	134	ILE	3.1
1	F	54	PHE	3.0
1	B	94	LYS	2.9
1	F	103	LEU	2.9
1	E	41	PHE	2.9
1	E	83	ALA	2.9
1	B	134	ILE	2.9
1	C	79	PHE	2.8
1	F	99	LEU	2.7
1	B	156	LEU	2.7
1	C	13	PHE	2.6
1	E	110	LEU	2.6
1	E	107	LEU	2.6
1	F	27	LYS	2.6
1	E	80	LEU	2.6
1	F	151	LEU	2.6
1	E	54	PHE	2.6
1	A	157	GLU	2.5
1	B	34	TYR	2.5
1	B	83	ALA	2.5
1	C	10	THR	2.5
1	F	107	LEU	2.5
1	F	121	THR	2.5
1	D	114	TYR	2.5
1	B	147	PHE	2.5
1	F	90	TYR	2.5
1	B	17	GLN	2.4
1	F	152	GLY	2.4
1	D	8	VAL	2.4
1	F	14	LEU	2.4
1	A	145	TRP	2.4
1	F	21	LEU	2.4
1	A	155	PRO	2.4
1	F	110	LEU	2.4
1	B	66	LEU	2.4
1	C	12	GLU	2.4
1	E	156	LEU	2.4
1	F	40	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	10	THR	2.3
1	F	31	ILE	2.3
1	B	155	PRO	2.3
1	B	107	LEU	2.3
1	A	67	ALA	2.3
1	D	35	MET	2.2
1	D	12	GLU	2.2
1	F	98	GLN	2.2
1	B	148	LYS	2.2
1	E	23	VAL	2.2
1	C	107	LEU	2.2
1	C	134	ILE	2.2
1	C	80	LEU	2.2
1	C	68	ILE	2.2
1	E	40	PHE	2.2
1	E	103	LEU	2.2
1	A	10	THR	2.1
1	F	34	TYR	2.1
1	B	79	PHE	2.1
1	F	8	VAL	2.1
1	E	147	PHE	2.1
1	C	147	PHE	2.0
1	D	145	TRP	2.0
1	B	91	THR	2.0

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	205	1/1	0.10	0.20	217,217,217,217	0
2	ZN	D	208	1/1	0.44	0.24	131,131,131,131	1
2	ZN	A	214	1/1	0.46	0.90	435,435,435,435	0
2	ZN	A	212	1/1	0.52	0.15	210,210,210,210	0
2	ZN	B	208	1/1	0.53	0.16	178,178,178,178	0
2	ZN	C	206	1/1	0.55	0.14	179,179,179,179	0
2	ZN	D	203	1/1	0.64	0.09	189,189,189,189	0
2	ZN	D	204	1/1	0.64	0.11	175,175,175,175	0
2	ZN	F	203	1/1	0.66	0.12	197,197,197,197	0
2	ZN	B	209	1/1	0.68	0.21	170,170,170,170	1
2	ZN	A	210	1/1	0.74	0.21	213,213,213,213	0
2	ZN	A	206	1/1	0.76	0.14	195,195,195,195	0
2	ZN	D	202	1/1	0.78	0.24	179,179,179,179	0
2	ZN	B	212	1/1	0.78	0.12	141,141,141,141	0
2	ZN	B	207	1/1	0.82	0.46	206,206,206,206	0
2	ZN	B	210	1/1	0.82	0.20	132,132,132,132	1
2	ZN	B	215	1/1	0.83	0.06	183,183,183,183	1
2	ZN	A	216	1/1	0.84	0.25	111,111,111,111	0
2	ZN	F	204	1/1	0.85	0.08	174,174,174,174	0
2	ZN	C	203	1/1	0.86	0.18	140,140,140,140	1
2	ZN	D	210	1/1	0.86	0.10	118,118,118,118	1
2	ZN	B	205	1/1	0.86	0.21	130,130,130,130	0
2	ZN	B	206	1/1	0.86	0.21	140,140,140,140	0
2	ZN	F	206	1/1	0.86	0.11	255,255,255,255	0
2	ZN	B	216	1/1	0.87	0.26	178,178,178,178	0
2	ZN	A	205	1/1	0.87	0.17	137,137,137,137	1
2	ZN	F	205	1/1	0.89	0.22	176,176,176,176	0
2	ZN	A	211	1/1	0.90	0.13	208,208,208,208	0
2	ZN	C	208	1/1	0.90	0.08	186,186,186,186	0
2	ZN	E	203	1/1	0.91	0.14	151,151,151,151	1
2	ZN	F	202	1/1	0.91	0.22	140,140,140,140	0
2	ZN	A	208	1/1	0.91	0.12	140,140,140,140	1
2	ZN	A	202	1/1	0.91	0.05	157,157,157,157	0
2	ZN	A	217	1/1	0.91	0.16	119,119,119,119	1
2	ZN	E	202	1/1	0.91	0.10	145,145,145,145	1
2	ZN	D	212	1/1	0.92	0.10	123,123,123,123	1
2	ZN	A	215	1/1	0.92	0.38	242,242,242,242	0
2	ZN	A	209	1/1	0.92	0.20	231,231,231,231	0
2	ZN	C	201	1/1	0.92	0.29	115,115,115,115	0
2	ZN	B	214	1/1	0.93	0.25	178,178,178,178	0
2	ZN	B	201	1/1	0.93	0.31	110,110,110,110	0
2	ZN	A	204	1/1	0.93	0.13	135,135,135,135	1
2	ZN	C	207	1/1	0.94	0.28	276,276,276,276	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	207	1/1	0.94	0.12	138,138,138,138	1
2	ZN	C	202	1/1	0.95	0.21	103,103,103,103	0
2	ZN	D	206	1/1	0.95	0.16	113,113,113,113	0
2	ZN	D	207	1/1	0.95	0.49	189,189,189,189	0
2	ZN	A	213	1/1	0.95	0.09	151,151,151,151	1
2	ZN	B	213	1/1	0.95	0.37	230,230,230,230	1
2	ZN	D	211	1/1	0.95	0.12	128,128,128,128	1
2	ZN	A	203	1/1	0.95	0.29	131,131,131,131	0
2	ZN	B	211	1/1	0.96	0.27	133,133,133,133	0
2	ZN	D	209	1/1	0.96	0.17	120,120,120,120	1
2	ZN	B	202	1/1	0.97	0.29	135,135,135,135	0
2	ZN	D	201	1/1	0.97	0.12	111,111,111,111	1
2	ZN	C	204	1/1	0.98	0.16	137,137,137,137	0
2	ZN	A	201	1/1	0.98	0.25	97,97,97,97	0
2	ZN	F	201	1/1	0.98	0.20	133,133,133,133	0
2	ZN	E	201	1/1	0.98	0.05	167,167,167,167	1
2	ZN	B	203	1/1	0.99	0.22	111,111,111,111	0
2	ZN	B	204	1/1	0.99	0.20	94,94,94,94	0
2	ZN	C	205	1/1	0.99	0.28	119,119,119,119	0

5.5 Other polymers (i)

There are no such residues in this entry.