



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5OT4 / pdb_00005ot4
Title : Structure of the Legionella pneumophila effector RidL (1-866)
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Deposited on : 2017-08-20
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

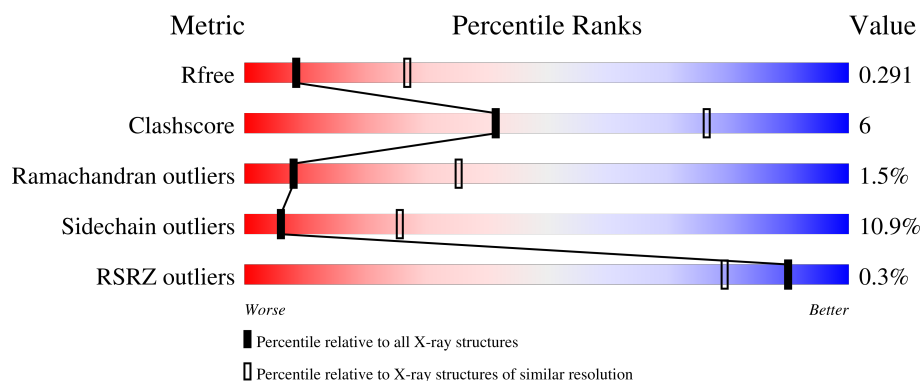
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	901	 73% 18% • 6%
1	B	901	 74% 17% • 7%
1	C	901	 63% 20% • 13%
1	D	901	 72% 18% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26232 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 Interaptin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	846	Total	C	N	O	S	0	0	0
			6687	4198	1164	1312	13			
1	B	842	Total	C	N	O	S	0	0	0
			6673	4191	1162	1306	14			
1	C	787	Total	C	N	O	S	0	0	0
			6238	3915	1084	1225	14			
1	D	836	Total	C	N	O	S	0	0	0
			6628	4158	1151	1305	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP G8UZ99
B	0	SER	-	expression tag	UNP G8UZ99
C	0	SER	-	expression tag	UNP G8UZ99
D	0	SER	-	expression tag	UNP G8UZ99

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		



MET	K747	D594	Q472	L355	T169	S0
HIS	P754	R597	L476	T362	E5	E5
TYR	VAL	S601	L482	K363	Y6	I7
TYR	HIS	S602	Q481	K364	V181	K13
ASN	LEU	H615	L482	A365	L182	E14
SER	TYR	H616	E490	V366	R195	F15
GLY	ASN	Q617	E490	T367	D196	
ILE	PRO	H618	V493	E368	L200	I22
LYS	THR	I619		E369		
LYS	PHI			N370	K27	K27
ARG	GLN		L508	L371	V39	V39
HIS	GLY	T626	L515	M378	L44	L44
PRO	THR	S627	L515	M379	F54	F54
PRO	ALA	N628	F518		I57	I57
VAL	ARG	N628		T386	V58	V58
SER	SER	L638	F518	K387	V240	V240
SER	LYS	L639	I521	D388	F64	F64
ASP	ALA		H522		W65	W65
GLN	A771	K643	N523	N391	D66	D66
ILE	Q772	T646	V526	L392	E67	E67
PRO	M773	F647	K534	K393	L72	L72
PRO				A394		
LEU	L786			L395		
PRO		I651	I537	D396		
ASN	L791	V652	T538	A397		
VAL			T539	L401		
PRO	L798	L656	N540	F410		
ASN		L657		V413		
PRO	L802	L539		L414		
ASN	K803	P658	Q543	L417		
SER		P658	V544	G78		
LEU		L659		E300		
ARG	P811	K660	T552	P301		
SER	LYS	T664	A554	T304		
	ALA	N676		A314		
	GLY		T560	Q315		
	LEU	E700	Y561	G316		
		I701	T562	V317		
		K702	Q563	L318		
		L710	Y567	V326		
			L570	I131		
		K719	A573	T331		
		T720	I574	Q332		
		A721	K575	N333		
		L725	T576	L334		
			S577	A337		
		S731	S578	N339		
		I732	K584	T348		
		K733	D585	E349		
		T736	F586	L350		
		I739	L592	P167		
		K745	N593	P168		
		L746				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	242.65Å 230.91Å 86.73Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	167.27 – 3.00 167.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (167.27-3.00) 99.7 (167.27-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.229 , 0.295 0.230 , 0.291	Depositor DCC
R_{free} test set	4953 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26232	wwPDB-VP
Average B, all atoms (Å ²)	125.0	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 39.85 % 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 2.9839e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL

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	0.74	0/6793	1.01	8/9163 (0.1%)
1	B	0.77	1/6777 (0.0%)	1.03	7/9130 (0.1%)
1	C	0.87	1/6330 (0.0%)	1.07	12/8523 (0.1%)
1	D	0.78	1/6729 (0.0%)	1.02	5/9067 (0.1%)
All	All	0.79	3/26629 (0.0%)	1.03	32/35883 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	LEU	CA-C	6.25	1.55	1.52
1	D	364	LYS	CA-C	6.12	1.58	1.53
1	C	170	ILE	CA-CB	5.85	1.57	1.54

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	SER	N-CA-C	6.76	120.40	110.59
1	B	104	PHE	N-CA-C	6.58	118.45	111.28
1	B	366	VAL	N-CA-C	6.14	118.48	109.63
1	B	82	GLY	N-CA-C	6.11	119.22	111.09
1	D	386	ILE	N-CA-CB	6.10	117.17	110.53

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	6687	0	6729	74	0
1	B	6673	0	6726	80	0
1	C	6238	0	6270	97	0
1	D	6628	0	6666	83	0
2	B	6	0	8	0	0
All	All	26232	0	26399	334	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 6.

The worst 5 of 334 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:D:229:ASN:HD21	1:D:238:ASN:HD22	1.19	0.88
1:C:365:ALA:HA	1:C:370:ASN:HD22	1.48	0.79
1:A:337:ALA:HB3	1:A:378:MET:HE1	1.64	0.78
1:C:212:LEU:HD23	1:C:231:LEU:HD11	1.65	0.78
1:C:229:ASN:HD21	1:C:238:ASN:HD21	1.33	0.76

There are no symmetry-related clashes.

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	842/901 (94%)	757 (90%)	74 (9%)	11 (1%)	9	38
1	B	838/901 (93%)	780 (93%)	50 (6%)	8 (1%)	12	45
1	C	775/901 (86%)	675 (87%)	78 (10%)	22 (3%)	4	21
1	D	828/901 (92%)	759 (92%)	60 (7%)	9 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3283/3604 (91%)	2971 (90%)	262 (8%)	50 (2%)	8	35

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	B	50	ASP
1	B	628	ASN
1	C	12	ASN
1	C	300	GLU

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	728/779 (94%)	648 (89%)	80 (11%)	6	25
1	B	726/779 (93%)	651 (90%)	75 (10%)	7	28
1	C	680/779 (87%)	590 (87%)	90 (13%)	4	18
1	D	725/779 (93%)	657 (91%)	68 (9%)	8	32
All	All	2859/3116 (92%)	2546 (89%)	313 (11%)	6	26

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	708	GLN
1	D	592	LEU
1	C	773	MET
1	D	355	LEU
1	D	725	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	204	ASN
1	D	229	ASN
1	C	210	GLN
1	C	555	ASN
1	D	385	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	1001	-	5,5,5	0.39	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1001	-	-	0/4/4/4	-

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.

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	846/901 (93%)	-0.60	6 (0%) 84 66	80, 116, 158, 196	0
1	B	842/901 (93%)	-0.69	0 100 100	78, 111, 156, 210	0
1	C	787/901 (87%)	-0.44	2 (0%) 90 79	80, 141, 193, 219	0
1	D	836/901 (92%)	-0.59	1 (0%) 92 86	69, 127, 174, 204	0
All	All	3311/3604 (91%)	-0.58	9 (0%) 90 79	69, 122, 177, 219	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	PHE	4.0
1	D	65	TRP	3.0
1	A	12	ASN	3.0
1	A	558	PRO	2.9
1	A	58	VAL	2.5

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 oligosaccharides in this entry.

6.4 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($\text{\AA}^2$)	Q<0.9
2	GOL	B	1001	6/6	0.88	0.12	155,167,170,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.