



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6B7P / pdb_00006b7p
Title : Crystal structure of Legionella effector sdeD (lpg2509)
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Deposited on : 2017-10-04
Resolution : 1.51 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 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
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

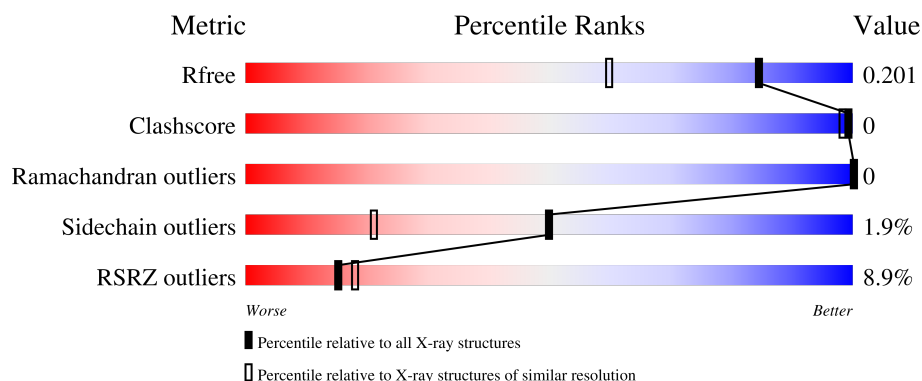
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	383	7% 69% 10% 21%
1	B	383	8% 68% 13% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5305 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 SdeD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	1	0
			2415	1535	411	456	13			
1	B	307	Total	C	N	O	S	0	1	0
			2442	1549	417	464	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q6RCQ7
A	1	MET	-	expression tag	UNP Q6RCQ7
B	0	SER	-	expression tag	UNP Q6RCQ7
B	1	MET	-	expression tag	UNP Q6RCQ7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	225	Total	O	0	0
			225	225		
2	B	223	Total	O	0	0
			223	223		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	154.35Å 154.35Å 89.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.00 – 1.51 44.00 – 1.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.00-1.51) 99.8 (44.00-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	50.00 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.168 , 0.194 0.178 , 0.201	Depositor DCC
R_{free} test set	6286 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.002 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.001 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.000 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.008 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.002 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.012 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5305	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	1.71	25/2476 (1.0%)	1.41	15/3354 (0.4%)
1	B	1.71	34/2504 (1.4%)	1.39	9/3392 (0.3%)
All	All	1.71	59/4980 (1.2%)	1.40	24/6746 (0.4%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	VAL	N-CA	7.34	1.53	1.46
1	B	35	ASN	C-O	-7.33	1.15	1.24
1	B	275	PRO	CA-C	7.04	1.61	1.52
1	B	284	THR	N-CA	6.98	1.54	1.46
1	B	29	GLY	C-O	-6.97	1.17	1.23
1	A	26	THR	CA-C	-6.84	1.43	1.52
1	A	74	ARG	C-O	-6.74	1.16	1.24
1	B	233	ALA	C-O	-6.61	1.16	1.24
1	B	183	TYR	C-O	-6.60	1.16	1.24
1	B	139	TYR	C-O	-6.55	1.16	1.24
1	B	130	GLY	C-O	-6.54	1.16	1.23
1	A	248	ASP	N-CA	6.39	1.54	1.46
1	A	158	GLU	C-O	-6.38	1.16	1.24
1	A	28	VAL	N-CA	6.22	1.53	1.46
1	B	224	GLN	N-CA	-6.20	1.39	1.46
1	A	26	THR	C-O	6.16	1.31	1.23
1	A	213	ILE	CA-C	6.16	1.60	1.52
1	B	55	ILE	CA-C	-6.14	1.45	1.52
1	B	87	LYS	N-CA	6.10	1.54	1.46
1	A	22	SER	C-O	5.99	1.31	1.24
1	A	53	ARG	CA-C	-5.95	1.45	1.52
1	B	34	TYR	C-O	-5.94	1.16	1.23
1	B	213	ILE	CA-C	5.92	1.60	1.52
1	A	121	ALA	C-O	-5.90	1.16	1.24
1	B	301	VAL	N-CA	-5.90	1.42	1.46
1	A	122	GLY	C-O	-5.84	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	LYS	C-O	5.83	1.30	1.24
1	B	301	VAL	CA-CB	5.74	1.59	1.53
1	A	263	GLN	CA-CB	5.68	1.62	1.53
1	A	219	HIS	CA-CB	-5.67	1.44	1.53
1	B	291	VAL	C-O	-5.67	1.17	1.24
1	B	284	THR	C-O	5.63	1.30	1.24
1	A	247	ILE	CA-C	5.62	1.59	1.52
1	A	155	LEU	CB-CG	-5.61	1.42	1.53
1	A	81	LEU	C-O	5.57	1.30	1.24
1	B	200	VAL	C-O	-5.48	1.18	1.24
1	B	224	GLN	CA-C	5.47	1.59	1.52
1	B	107	LEU	CA-C	5.44	1.59	1.52
1	B	295	TYR	C-O	-5.41	1.17	1.24
1	B	51	LEU	N-CA	5.41	1.53	1.46
1	B	11	GLU	CA-C	5.39	1.59	1.52
1	A	228	ASP	CA-C	5.37	1.59	1.52
1	B	4	ILE	N-CA	-5.36	1.39	1.46
1	B	147	TYR	C-O	-5.35	1.17	1.24
1	B	82	MET	N-CA	-5.31	1.39	1.46
1	B	298	LEU	C-O	-5.26	1.18	1.24
1	A	175	SER	C-O	-5.21	1.17	1.23
1	B	135	ARG	C-O	-5.21	1.18	1.24
1	B	300	SER	N-CA	5.20	1.53	1.46
1	A	148	ALA	N-CA	5.19	1.52	1.46
1	B	234	ARG	C-O	-5.19	1.18	1.24
1	A	264	ARG	C-O	-5.19	1.18	1.24
1	B	63	HIS	CA-CB	-5.07	1.45	1.53
1	B	146	GLU	C-O	-5.07	1.18	1.24
1	A	172	VAL	C-O	-5.07	1.19	1.24
1	B	176	PHE	N-CA	-5.06	1.40	1.46
1	A	166	ARG	C-O	-5.05	1.17	1.24
1	B	228	ASP	CA-C	5.03	1.59	1.52
1	A	219	HIS	N-CA	5.01	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	VAL	CA-C-O	7.19	123.39	119.15
1	A	14	GLU	CB-CG-CD	6.67	123.95	112.60
1	B	64	ARG	CB-CA-C	6.56	116.87	110.71
1	B	101	ILE	O-C-N	6.54	128.47	121.87
1	A	213	ILE	CB-CG1-CD1	6.21	126.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	SER	O-C-N	6.16	126.22	121.23
1	B	109	LEU	O-C-N	-6.06	115.12	122.22
1	A	23	GLN	CA-C-O	6.05	126.05	120.60
1	A	262	VAL	O-C-N	-5.86	116.17	121.91
1	A	55	ILE	O-C-N	-5.82	116.87	123.10
1	B	231	HIS	N-CA-C	5.62	117.40	111.28
1	B	6	ASP	N-CA-C	5.51	117.02	110.19
1	A	144	PHE	CA-C-O	-5.46	115.07	120.70
1	B	220	LEU	N-CA-C	5.37	117.21	111.36
1	B	221	PHE	O-C-N	5.32	128.48	122.20
1	A	98	GLY	CA-C-O	5.29	124.99	119.06
1	A	125	SER	CA-C-O	-5.29	115.48	121.25
1	A	154	HIS	N-CA-C	5.19	119.23	113.01
1	A	307	TYR	CA-C-O	-5.17	112.01	120.80
1	A	154	HIS	CA-C-O	5.06	125.63	119.05
1	A	32	TRP	O-C-N	-5.05	116.08	122.19
1	A	263	GLN	N-CA-C	5.05	116.78	111.28
1	A	26	THR	CA-C-O	-5.04	113.57	118.97
1	B	77	MET	O-C-N	-5.03	116.41	122.15

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	2415	0	2344	0	0
1	B	2442	0	2361	2	0
2	A	225	0	0	0	0
2	B	223	0	0	0	0
All	All	5305	0	4705	2	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 0.

All (2) 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:B:252:TRP:N	1:B:253:PRO:CD	2.78	0.46
1:B:198:SER:HB2	1:B:199:PRO:HD2	2.03	0.40

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	300/383 (78%)	295 (98%)	5 (2%)	0	100	100
1	B	304/383 (79%)	300 (99%)	4 (1%)	0	100	100
All	All	604/766 (79%)	595 (98%)	9 (2%)	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	261/338 (77%)	256 (98%)	5 (2%)	50	21
1	B	264/338 (78%)	259 (98%)	5 (2%)	50	21
All	All	525/676 (78%)	515 (98%)	10 (2%)	50	21

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	128	SER
1	A	146	GLU
1	A	210	VAL
1	A	282	LYS
1	B	197	LYS
1	B	210	VAL
1	B	211	SER
1	B	259	LEU
1	B	264	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	254	HIS
1	A	277	GLN
1	B	23	GLN
1	B	143	GLN
1	B	224	GLN

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](#)

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	303/383 (79%)	0.49	25 (8%) 17 20	10, 21, 40, 72	1 (0%)
1	B	307/383 (80%)	0.62	29 (9%) 14 16	13, 23, 46, 84	1 (0%)
All	All	610/766 (79%)	0.56	54 (8%) 15 18	10, 22, 44, 84	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	VAL	8.0
1	A	210	VAL	7.8
1	B	209	GLY	7.4
1	B	259	LEU	5.7
1	A	36	TYR	5.2
1	B	39	PRO	4.5
1	B	308	GLU	4.2
1	A	35	ASN	4.1
1	B	207	SER	4.1
1	B	38	ASN	4.1
1	B	261	ARG	4.0
1	A	122	GLY	3.9
1	B	260	SER	3.7
1	B	254	HIS	3.6
1	A	41	ALA	3.5
1	A	205	GLY	3.3
1	B	37	LYS	3.2
1	B	1	MET	3.2
1	B	90	PRO	3.2
1	B	40	THR	3.1
1	A	175	SER	3.1
1	A	259	LEU	3.0
1	B	154	HIS	2.9
1	B	257	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLY	2.8
1	B	258	ASP	2.8
1	B	253	PRO	2.8
1	B	266	LEU	2.7
1	A	1	MET	2.6
1	B	35	ASN	2.6
1	B	262	VAL	2.6
1	A	193	LEU	2.6
1	A	211	SER	2.5
1	B	264	ARG	2.5
1	B	196	CYS	2.5
1	A	196	CYS	2.4
1	A	58	ASP	2.4
1	A	260	SER	2.4
1	A	6	ASP	2.4
1	A	128	SER	2.4
1	A	261	ARG	2.4
1	A	38	ASN	2.4
1	B	267	SER	2.3
1	A	264	ARG	2.2
1	A	258	ASP	2.2
1	B	274	VAL	2.2
1	B	91	SER	2.1
1	B	211	SER	2.1
1	B	59	GLY	2.1
1	A	37	LYS	2.1
1	A	224	GLN	2.1
1	A	131	ASP	2.1
1	A	39	PRO	2.0
1	B	273	ASN	2.0

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 oligosaccharides 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.