



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 09:58 PM UTC

PDB ID : 4Y17 / pdb_00004y17
Title : SdiA in complex with 3-oxo-C8-homoserine lactone
Authors : Nguyen, N.X.; Nguyen, Y.; Sperandio, V.; Jiang, Y.
Deposited on : 2015-02-06
Resolution : 2.84 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	:	FAILED
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

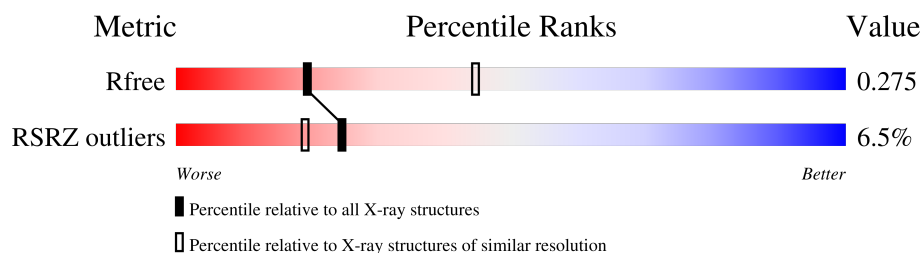
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11647 atoms, of which 5715 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.

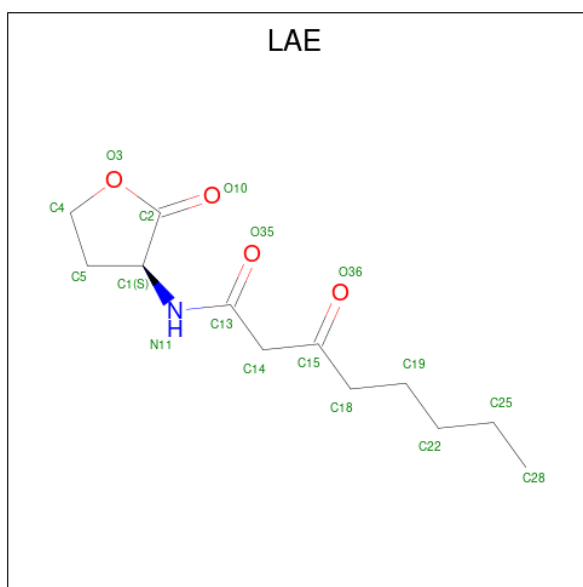
- Molecule 1 is a protein called Transcriptional regulator of ftsQAZ gene cluster.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	238	Total	C	H	N	O	S	0	0	0
			3839	1241	1894	339	351	14			
1	B	237	Total	C	H	N	O	S	0	0	0
			3841	1240	1901	336	350	14			
1	C	243	Total	C	H	N	O	S	0	0	0
			3908	1265	1920	349	360	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	HIS	-	expression tag	UNP Q8XBD0
A	242	HIS	-	expression tag	UNP Q8XBD0
A	243	HIS	-	expression tag	UNP Q8XBD0
A	244	HIS	-	expression tag	UNP Q8XBD0
A	245	HIS	-	expression tag	UNP Q8XBD0
A	246	HIS	-	expression tag	UNP Q8XBD0
B	241	HIS	-	expression tag	UNP Q8XBD0
B	242	HIS	-	expression tag	UNP Q8XBD0
B	243	HIS	-	expression tag	UNP Q8XBD0
B	244	HIS	-	expression tag	UNP Q8XBD0
B	245	HIS	-	expression tag	UNP Q8XBD0
B	246	HIS	-	expression tag	UNP Q8XBD0
C	241	HIS	-	expression tag	UNP Q8XBD0
C	242	HIS	-	expression tag	UNP Q8XBD0
C	243	HIS	-	expression tag	UNP Q8XBD0
C	244	HIS	-	expression tag	UNP Q8XBD0
C	245	HIS	-	expression tag	UNP Q8XBD0
C	246	HIS	-	expression tag	UNP Q8XBD0

- Molecule 2 is 3-OXO-OCTANOIC ACID (2-OXO-TETRAHYDRO-FURAN-3-YL)-AMIDE (CCD ID: LAE) (formula: C₁₂H₁₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	12	1	4		
2	B	1	Total	C	N	O	0	0
			17	12	1	4		
2	C	1	Total	C	N	O	0	0
			17	12	1	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		
3	C	1	Total	O	0	0
			1	1		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.49Å 92.43Å 119.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.47 – 2.84 41.47 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.47-2.84) 99.4 (41.47-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.234 , 0.271 0.240 , 0.275	Depositor DCC
R_{free} test set	1181 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11647	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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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 oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

3 ligands are 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	LAE	A	301	-	17,17,17	2.24	5 (29%)	17,21,21	1.85	5 (29%)
2	LAE	C	301	-	17,17,17	2.28	5 (29%)	17,21,21	1.63	5 (29%)
2	LAE	B	301	-	17,17,17	2.27	5 (29%)	17,21,21	2.18	4 (23%)

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	LAE	A	301	-	-	6/13/23/23	0/1/1/1
2	LAE	C	301	-	-	5/13/23/23	0/1/1/1
2	LAE	B	301	-	-	3/13/23/23	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	LAE	O3-C2	6.22	1.48	1.35
2	A	301	LAE	O3-C2	6.09	1.48	1.35
2	B	301	LAE	O3-C2	5.99	1.47	1.35
2	C	301	LAE	C13-N11	4.01	1.42	1.34
2	A	301	LAE	O3-C4	-3.97	1.36	1.46
2	B	301	LAE	C13-N11	3.94	1.42	1.34
2	B	301	LAE	O3-C4	-3.89	1.36	1.46
2	C	301	LAE	O3-C4	-3.87	1.36	1.46
2	A	301	LAE	C13-N11	3.84	1.42	1.34
2	B	301	LAE	C1-C2	-3.31	1.45	1.52
2	A	301	LAE	C1-C2	-2.93	1.46	1.52
2	C	301	LAE	C1-C2	-2.92	1.46	1.52
2	B	301	LAE	C1-N11	-2.85	1.39	1.45
2	C	301	LAE	C1-N11	-2.83	1.40	1.45
2	A	301	LAE	C1-N11	-2.79	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	LAE	O3-C2-O10	5.08	126.82	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	LAE	O3-C2-O10	4.41	126.12	121.43
2	B	301	LAE	C4-O3-C2	-4.16	106.63	110.35
2	C	301	LAE	O3-C2-O10	3.97	125.65	121.43
2	A	301	LAE	C4-O3-C2	-3.68	107.06	110.35
2	B	301	LAE	C5-C1-N11	-3.37	107.86	115.03
2	B	301	LAE	C14-C13-N11	2.83	121.15	116.31
2	C	301	LAE	C5-C1-N11	-2.35	110.03	115.03
2	A	301	LAE	C14-C13-N11	2.35	120.33	116.31
2	A	301	LAE	C5-C1-N11	-2.14	110.49	115.03
2	C	301	LAE	C14-C13-N11	2.14	119.96	116.31
2	C	301	LAE	C4-O3-C2	-2.13	108.44	110.35
2	C	301	LAE	C19-C18-C15	-2.12	109.21	114.59
2	A	301	LAE	O35-C13-N11	-2.12	119.37	122.95

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	LAE	C13-C14-C15-C18
2	A	301	LAE	C13-C14-C15-O36
2	A	301	LAE	C14-C15-C18-C19
2	A	301	LAE	O36-C15-C18-C19
2	C	301	LAE	N11-C13-C14-C15
2	C	301	LAE	O35-C13-C14-C15
2	B	301	LAE	C15-C18-C19-C22
2	A	301	LAE	C19-C22-C25-C28
2	C	301	LAE	O36-C15-C18-C19
2	C	301	LAE	C14-C15-C18-C19
2	A	301	LAE	C18-C19-C22-C25
2	B	301	LAE	C14-C15-C18-C19
2	B	301	LAE	O36-C15-C18-C19
2	C	301	LAE	C15-C18-C19-C22

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	238/246 (96%)	0.32	14 (5%) 28 21	46, 71, 122, 192	0
1	B	237/246 (96%)	0.19	8 (3%) 48 38	46, 69, 106, 168	0
1	C	243/246 (98%)	0.80	25 (10%) 12 9	54, 99, 156, 259	0
All	All	718/738 (97%)	0.44	47 (6%) 25 19	46, 78, 142, 259	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	GLU	6.4
1	A	142	GLU	5.5
1	A	143	ILE	4.9
1	A	144	PRO	4.9
1	C	145	ILE	4.1
1	C	241	HIS	4.1
1	B	141	ARG	4.0
1	B	143	ILE	3.9
1	C	6	PHE	3.5
1	C	12	THR	3.5
1	A	140	ALA	3.4
1	C	244	HIS	3.3
1	B	140	ALA	3.3
1	B	241	HIS	3.3
1	C	17	PHE	3.2
1	A	145	ILE	3.0
1	A	141	ARG	2.9
1	C	222	ILE	2.9
1	C	143	ILE	2.9
1	C	142	GLU	2.9
1	C	10	ARG	2.9
1	A	6	PHE	2.8
1	C	146	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	7	PHE	2.8
1	C	144	PRO	2.8
1	C	240	ILE	2.8
1	C	141	ARG	2.7
1	C	15	LEU	2.7
1	C	5	ASP	2.7
1	C	221	LYS	2.7
1	B	139	SER	2.6
1	A	242	HIS	2.5
1	C	2	GLN	2.5
1	A	146	LEU	2.4
1	A	7	PHE	2.4
1	B	107	TRP	2.4
1	C	140	ALA	2.3
1	C	14	LEU	2.3
1	C	139	SER	2.3
1	C	223	ASN	2.3
1	C	9	TRP	2.3
1	A	138	CYS	2.2
1	B	101	ASN	2.2
1	A	11	ARG	2.1
1	A	139	SER	2.1
1	C	8	SER	2.1
1	A	176	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	LAE	C	301	17/17	0.88	0.22	71,75,81,83	0
2	LAE	B	301	17/17	0.90	0.20	53,63,71,76	0
2	LAE	A	301	17/17	0.94	0.13	48,55,62,65	0

5.5 Other polymers [i](#)

There are no such residues in this entry.