

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 17, 2022 – 06:08 PM JST

PDB ID	:	7V5V
Title	:	LysR family transcriptional regulator RipR from Salmonella Typhimurium
Authors	:	Ki, N.; Ha, NC.
Deposited on	:	2021-08-18
Resolution	:	2.37  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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.37 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\# { m Entries,\ resolution\ range}({ m \AA}))$		
$R_{free}$	130704	5509(2.40-2.36)		
Clashscore	141614	6082(2.40-2.36)		
Ramachandran outliers	138981	5973 (2.40-2.36)		
Sidechain outliers	138945	5975 (2.40-2.36)		
RSRZ outliers	127900	5397(2.40-2.36)		

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 <=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	А	208	8%	12%	•
1	В	208	86%	12%	•
1	С	208	3% 82%	14%	••
1	D	208	78%	19%	••



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6309 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	207	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	207	1580	1008	275	290	$\overline{7}$	0	0	U
1	D	207	Total	С	Ν	0	S	0	0	0
	D	207	1584	1011	275	290	8			
1	С	203	Total	С	Ν	0	S	0	0	0
			1551	992	268	284	7			0
1 D	205	Total	$\mathbf{C}$	Ν	0	$\mathbf{S}$	0	0	0	
	205	1564	999	270	288	$\overline{7}$		0	U	

• Molecule 1 is a protein called RipR.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	85	MET	-	initiating methionine	UNP Q93DX4
В	85	MET	-	initiating methionine	UNP Q93DX4
С	85	MET	-	initiating methionine	UNP Q93DX4
D	85	MET	-	initiating methionine	UNP Q93DX4

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	4	Total O 4 4	0	0
2	В	10	Total         O           10         10	0	0
2	С	8	Total O 8 8	0	0
2	D	8	Total O 8 8	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: RipR



# V255 MET V235 MET P235 ALA V231 R34 V231 R34 S236 ALA S236 ALA S236 ALA S236 ALA S236 ALA S236 ALA S100 S100 S265 ALA R249 P108 R112 R112 V264 R116 V275 L147 V265 L147 V265 L147 V265 L146 V265 L147 V279 R166 L279 R166 L279 R166 L162 R166 L163 R161 L279 L147 D263 R161 L279 L162 R166 L163 R166 L163 R166 L163 R161 <



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	66.41Å 72.42Å 91.61Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $104.62^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Posclution}(\mathbf{\hat{A}})$	39.26 - 2.37	Depositor
Resolution (A)	39.26 - 2.37	EDS
% Data completeness	95.8 (39.26-2.37)	Depositor
(in resolution range)	95.8(39.26-2.37)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.50 (at 2.37 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
P. P.	0.236 , $0.295$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.235 , $0.289$	DCC
$R_{free}$ test set	1575 reflections $(4.81%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.4	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, $32.9$	EDS
L-test for $twinning^2$	$ L  > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6309	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.64% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.40	0/1607	0.56	0/2176	
1	В	0.32	0/1611	0.51	0/2181	
1	С	0.43	0/1578	0.58	2/2138~(0.1%)	
1	D	0.74	0/1591	0.73	3/2155~(0.1%)	
All	All	0.50	0/6387	0.60	5/8650~(0.1%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	D	251	VAL	N-CA-C	-9.34	85.77	111.00
1	D	251	VAL	CB-CA-C	9.08	128.66	111.40
1	С	251	VAL	N-CA-C	-6.05	94.66	111.00
1	С	251	VAL	CB-CA-C	5.34	121.54	111.40
1	D	154	ASN	N-CA-CB	5.15	119.88	110.60

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	А	1580	0	1628	13	0
1	В	1584	0	1634	12	0
1	С	1551	0	1601	18	2
1	D	1564	0	1610	19	2



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	4	0	0	0	0
2	В	10	0	0	0	0
2	С	8	0	0	0	0
2	D	8	0	0	0	0
All	All	6309	0	6473	58	2

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 5.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:238:GLU:O	1:C:115:LYS:NZ	2.12	0.83
1:D:193:PHE:O	1:D:222:GLY:N	2.12	0.82
1:D:162:LEU:HD11	1:D:272:LEU:HB2	1.63	0.80
1:C:202:LEU:N	1:C:202:LEU:HD23	1.97	0.78
1:D:249:ARG:O	1:D:251:VAL:O	2.06	0.73
1:C:130:THR:HG23	1:C:147:LEU:HB2	1.73	0.71
1:D:208:VAL:HA	1:D:243:MET:HE2	1.77	0.66
1:C:138:ASN:HD21	1:C:156:ARG:HG3	1.62	0.65
1:A:127:GLU:OE2	1:D:227:GLN:NE2	2.29	0.62
1:C:202:LEU:HD23	1:C:202:LEU:H	1.64	0.60
1:A:254:LYS:HA	1:A:254:LYS:HE3	1.84	0.59
1:A:238:GLU:OE2	1:D:116:ARG:NH2	2.36	0.58
1:C:232:ILE:HD11	1:C:244:VAL:HG11	1.86	0.57
1:B:193:PHE:HB3	1:B:195:LEU:HD23	1.87	0.56
1:D:104:ASN:O	1:D:108:PRO:HD2	2.06	0.55
1:C:156:ARG:HA	1:C:156:ARG:NE	2.22	0.55
1:D:156:ARG:O	1:D:156:ARG:HG2	2.08	0.54
1:C:169:ILE:HD13	1:C:243:MET:HG3	1.89	0.54
1:B:130:THR:HG23	1:B:147:LEU:HB2	1.91	0.53
1:C:113:THR:HG22	1:C:289:LYS:HD3	1.91	0.53
1:A:193:PHE:HB3	1:A:195:LEU:HD13	1.90	0.53
1:C:148:ARG:HD2	1:C:204:LEU:HD13	1.89	0.52
1:B:99:ALA:HB2	1:C:227:GLN:NE2	2.24	0.52
1:C:165:GLU:HG2	1:C:268:ALA:HB3	1.92	0.51
1:D:94:ARG:HB3	1:D:142:LEU:HD23	1.93	0.50
1:B:151:PHE:CD1	1:B:151:PHE:N	2.72	0.50
1:D:275:ARG:NH1	1:D:278:ASP:OD2	2.43	0.50
1:A:130:THR:HG23	1:A:147:LEU:HB2	1.92	0.50
1:A:95:VAL:HG13	1:A:144:VAL:HG13	1.96	0.47



A 4 amo 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:165:GLU:OE2	1:A:247:SER:N	2.47	0.47
1:B:151:PHE:H	1:B:151:PHE:HD1	1.57	0.47
1:A:211:ALA:HA	1:A:264:GLN:OE1	2.14	0.47
1:C:162:LEU:HD11	1:C:272:LEU:HB2	1.96	0.47
1:B:232:ILE:HG23	1:B:256:VAL:HG11	1.98	0.46
1:B:175:HIS:NE2	1:B:191:GLU:OE2	2.46	0.46
1:D:108:PRO:O	1:D:112:ARG:HB2	2.15	0.46
1:C:151:PHE:HA	1:C:202:LEU:HD13	1.99	0.45
1:C:94:ARG:NH1	1:C:140:GLY:O	2.49	0.44
1:C:182:GLN:HB2	1:C:262:ALA:HB2	1.99	0.44
1:D:130:THR:HG23	1:D:147:LEU:HB2	1.98	0.44
1:A:122:ARG:HE	1:A:122:ARG:HB3	1.50	0.43
1:B:142:LEU:O	1:B:275:ARG:NH1	2.41	0.43
1:D:100:SER:HB3	1:D:228:ILE:HD12	2.01	0.42
1:A:165:GLU:OE2	1:A:247:SER:HB3	2.19	0.42
1:B:154:ASN:OD1	1:B:154:ASN:N	2.53	0.42
1:D:210:LYS:HD3	1:D:214:LYS:HE3	2.02	0.42
1:A:204:LEU:HD12	1:A:204:LEU:N	2.35	0.41
1:A:92:VAL:CG2	1:A:122:ARG:HH21	2.33	0.41
1:D:263:ASP:OD1	1:D:263:ASP:N	2.54	0.41
1:D:225:VAL:HG12	1:D:231:VAL:HG23	2.02	0.41
1:D:192:PHE:HA	1:D:220:LYS:O	2.21	0.41
1:B:204:LEU:O	1:B:208:VAL:HG23	2.21	0.41
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.87	0.41
1:D:221:ILE:H	1:D:221:ILE:HD12	1.86	0.41
1:D:205:TYR:CD1	1:D:205:TYR:C	2.94	0.40
1:B:276:ARG:HE	1:B:276:ARG:HB2	1.66	0.40
1:C:210:LYS:HD2	1:C:210:LYS:N	2.35	0.40
1:A:104:ASN:O	1:A:108:PRO:HD2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:NH2	$1:D:221:ILE:O[2_645]$	1.72	0.48
1:C:289:LYS:O	1:D:181:LYS:NZ[1_545]	1.92	0.28



### 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	Perce	$\mathbf{ntiles}$
1	А	205/208~(99%)	200~(98%)	5(2%)	0	100	100
1	В	205/208~(99%)	199~(97%)	6 (3%)	0	100	100
1	С	201/208~(97%)	197~(98%)	4 (2%)	0	100	100
1	D	203/208~(98%)	196~(97%)	7 (3%)	0	100	100
All	All	814/832~(98%)	792 (97%)	22 (3%)	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	Perce	entiles
1	А	170/171~(99%)	158~(93%)	12 (7%)	14	21
1	В	171/171~(100%)	156~(91%)	15 (9%)	10	13
1	С	168/171~(98%)	160~(95%)	8 (5%)	25	39
1	D	169/171~(99%)	157~(93%)	12 (7%)	14	21
All	All	678/684~(99%)	631~(93%)	47 (7%)	15	22

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	141	SER
1	А	147	LEU



Mol	Chain	Res	Type
1	А	155	GLU
1	А	160	ARG
1	А	195	LEU
1	А	196	PHE
1	А	202	LEU
1	А	203	SER
1	А	223	GLN
1	А	236	SER
1	А	252	ASN
1	А	267	VAL
1	В	85	MET
1	В	90	SER
1	В	115	LYS
1	В	151	PHE
1	В	154	ASN
1	В	159	LEU
1	В	163	SER
1	В	173	GLU
1	В	182	GLN
1	В	186	SER
1	В	195	LEU
1	В	196	PHE
1	В	198	ARG
1	В	203	SER
1	В	236	SER
1	С	90	SER
1	С	115	LYS
1	С	116	ARG
1	С	157	PHE
1	C	181	LYS
1	C	202	LEU
1	C	254	LYS
1	C	289	LYS
1	D	89	GLU
1	D	126	GLU
1	D	154	ASN
1	D	160	ARG
1	D	167	MET
1	D	186	SER
1	D	200	ILE
1	D	204	LEU
1	D	210	LYS



Continued from previous page...

Mol	Chain	Res	Type
1	D	236	SER
1	D	254	LYS
1	D	265	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	252	ASN
1	В	252	ASN
1	С	129	ASN
1	D	158	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 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,  $95^{th}$  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	А	207/208~(99%)	0.90	17 (8%) 11 12	27, 40, 61, 159	0
1	В	207/208~(99%)	0.91	22 (10%) 6 7	26, 39, 63, 113	0
1	С	203/208~(97%)	0.68	6 (2%) 50 53	24, 37, 55, 71	0
1	D	205/208~(98%)	0.72	9 (4%) 34 37	23, 34, 54, 122	0
All	All	822/832~(98%)	0.80	54 (6%) 18 20	23, 38, 59, 159	0

All (54) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	163	SER	5.4
1	В	291	THR	4.8
1	D	159	LEU	4.8
1	D	222	GLY	4.7
1	D	221	ILE	4.2
1	А	203	SER	4.1
1	А	292	GLY	3.9
1	D	154	ASN	3.8
1	В	86	ALA	3.7
1	В	155	GLU	3.6
1	С	152	THR	3.6
1	С	156	ARG	3.5
1	А	156	ARG	3.2
1	С	216	GLY	3.0
1	В	88	GLY	2.9
1	А	155	GLU	2.8
1	А	88	GLY	2.7
1	С	120	ASP	2.7
1	А	291	THR	2.7
1	В	158	GLN	2.7
1	С	163	SER	2.6



Mol	Chain	Res	Type	RSRZ
1	В	177	ALA	2.6
1	D	279	THR	2.6
1	В	201	GLY	2.6
1	А	222	GLY	2.6
1	В	156	ARG	2.5
1	В	139	GLU	2.5
1	В	147	LEU	2.5
1	С	196	PHE	2.5
1	А	270	LEU	2.5
1	D	283	LEU	2.5
1	D	158	GLN	2.4
1	А	86	ALA	2.4
1	В	179	ALA	2.4
1	В	180	CYS	2.4
1	D	251	VAL	2.3
1	В	94	ARG	2.3
1	В	153	GLY	2.3
1	А	122	ARG	2.3
1	В	141	SER	2.3
1	В	174	THR	2.2
1	А	89	GLU	2.2
1	А	158	GLN	2.2
1	А	162	LEU	2.2
1	D	163	SER	2.2
1	В	178	ALA	2.2
1	В	200	ILE	2.2
1	A	194	LEU	2.1
1	В	171	LEU	2.1
1	А	207	ALA	2.1
1	В	137	LEU	2.1
1	В	154	ASN	2.0
1	A	172	ALA	2.0
1	В	182	GLN	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.

