



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2024 – 06:04 pm GMT

PDB ID : 7ZTB
Title : Structure of the Salmonella tRNA pyrophosphokinase CapRel
Authors : Garcia-Pino, A.
Deposited on : 2022-05-09
Resolution : 2.31 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

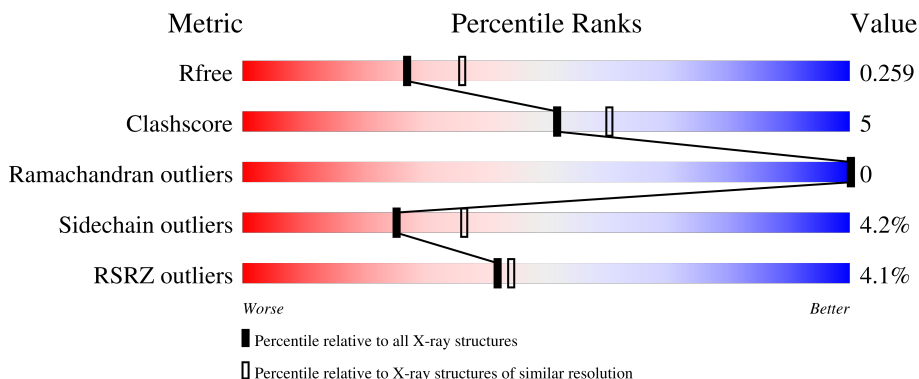
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.31 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	373	
1	B	373	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5534 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 RelA/SpoT family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2692	1704	473	504	11			
1	B	343	Total	C	N	O	S	0	0	0
			2612	1653	457	492	10			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

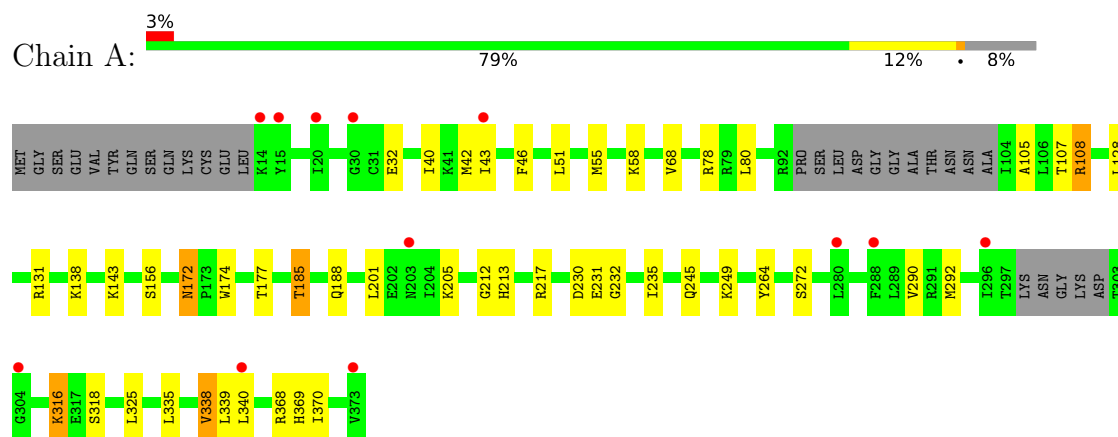
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	95	Total	O	0	0
			95	95		

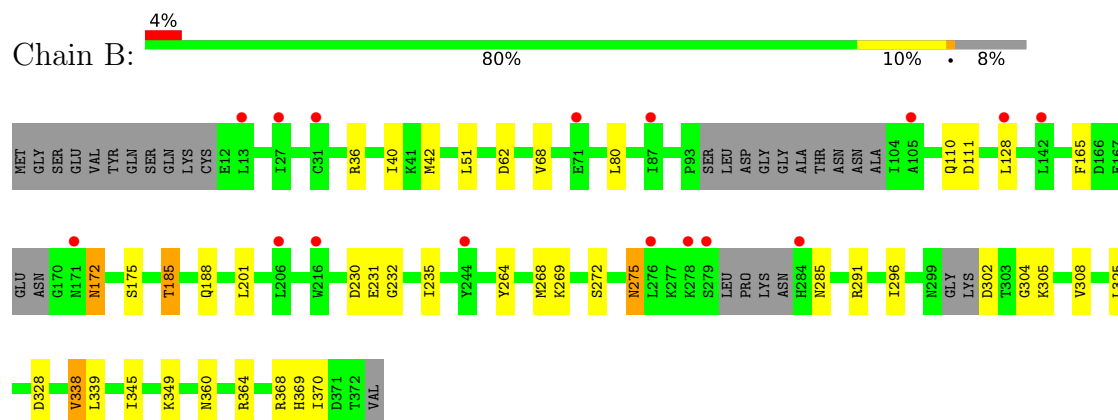
3 Residue-property plots [i](#)

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: RelA/SpoT family protein



• Molecule 1: RelA/SpoT family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.57Å 136.20Å 57.78Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	68.10 – 2.31 68.10 – 2.31	Depositor EDS
% Data completeness (in resolution range)	63.9 (68.10-2.31) 63.9 (68.10-2.31)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.10.4 (3-FEB-2022)	Depositor
R, R_{free}	0.212 , 0.265 0.203 , 0.259	Depositor DCC
R_{free} test set	1644 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5534	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA

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	0.44	0/2735	0.59	0/3686
1	B	0.39	0/2654	0.56	0/3591
All	All	0.41	0/5389	0.58	0/7277

There are no bond length outliers.

There are no bond angle outliers.

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	2692	0	2669	29	0
1	B	2612	0	2497	23	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	132	0	0	2	0
4	B	95	0	0	1	0
All	All	5534	0	5166	52	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 5.

All (52) 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:A:245:GLN:HE21	1:A:369:HIS:HD2	1.29	0.81
1:A:201:LEU:HD12	1:A:264:TYR:HB3	1.73	0.71
1:A:201:LEU:HD22	1:A:340:LEU:HD22	1.75	0.69
1:A:172:ASN:HD22	1:A:174:TRP:H	1.46	0.64
1:A:105:ALA:HB3	1:A:108:ARG:HG3	1.80	0.63
1:A:245:GLN:HE21	1:A:369:HIS:CD2	2.14	0.62
1:B:201:LEU:HD12	1:B:264:TYR:HB3	1.80	0.62
1:B:275:ASN:HD22	1:B:275:ASN:H	1.52	0.58
1:B:68:VAL:HG21	1:B:128:LEU:HA	1.86	0.57
1:B:368:ARG:HD2	4:B:508:HOH:O	2.05	0.56
1:A:212:GLY:O	1:A:217:ARG:HD2	2.05	0.55
1:A:51:LEU:O	1:A:55:MET:HG3	2.07	0.55
1:A:68:VAL:HG23	1:A:131:ARG:HD2	1.89	0.55
1:A:292:MET:HE2	1:A:335:LEU:HB2	1.91	0.52
1:B:264:TYR:O	1:B:268:MET:HG3	2.09	0.52
1:B:370:ILE:HG22	1:B:370:ILE:O	2.09	0.52
1:A:368:ARG:HD2	4:A:501:HOH:O	2.10	0.52
1:B:230:ASP:OD2	1:B:369:HIS:HE1	1.94	0.51
1:B:172:ASN:HB3	1:B:175:SER:HB2	1.92	0.50
1:B:264:TYR:CE1	1:B:338:VAL:HG11	2.46	0.49
1:B:165:PHE:HB2	1:B:175:SER:HA	1.94	0.49
1:A:325:LEU:HD22	1:A:339:LEU:HB2	1.95	0.49
1:A:316:LYS:HB2	1:A:316:LYS:HE2	1.75	0.48
1:B:325:LEU:HD22	1:B:339:LEU:HB2	1.96	0.47
1:A:185:THR:HG21	1:A:231:GLU:OE1	2.14	0.47
1:A:143:LYS:NZ	4:A:503:HOH:O	2.48	0.47
1:A:201:LEU:CD1	1:A:264:TYR:HB3	2.43	0.46
1:B:291:ARG:HD3	1:B:328:ASP:OD2	2.15	0.46
1:B:201:LEU:CD1	1:B:264:TYR:HB3	2.43	0.46
1:B:345:ILE:CG2	1:B:349:LYS:HE3	2.46	0.46
1:B:302:ASP:HA	1:B:305:LYS:HD3	1.97	0.45
1:A:213:HIS:O	1:A:217:ARG:HG3	2.17	0.45
1:A:249:LYS:HA	1:A:370:ILE:HG12	1.98	0.45
1:A:58:LYS:HG3	1:A:78:ARG:HB3	1.99	0.44
1:B:296:ILE:HA	1:B:304:GLY:HA2	1.99	0.44
1:A:290:VAL:HB	1:A:338:VAL:HG12	2.00	0.44
1:A:205:LYS:HD3	1:A:205:LYS:HA	1.85	0.44
1:A:51:LEU:HD13	1:A:80:LEU:HD22	2.00	0.44
1:B:185:THR:HG22	1:B:188:GLN:H	1.83	0.43
1:A:40:ILE:HA	1:A:43:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG21	1:A:128:LEU:HA	2.01	0.43
1:A:185:THR:CG2	1:A:231:GLU:OE1	2.67	0.43
1:B:51:LEU:HD13	1:B:80:LEU:HD22	2.00	0.42
1:B:360:ASN:O	1:B:364:ARG:HG3	2.20	0.42
1:A:185:THR:HG22	1:A:188:GLN:H	1.84	0.42
1:B:36:ARG:O	1:B:40:ILE:HG12	2.20	0.42
1:B:185:THR:HG21	1:B:231:GLU:OE1	2.20	0.42
1:A:46:PHE:CZ	1:A:107:THR:HA	2.54	0.42
1:A:232:GLY:HA2	1:A:235:ILE:HD11	2.01	0.42
1:B:232:GLY:HA2	1:B:235:ILE:HD11	2.00	0.42
1:A:230:ASP:OD2	1:A:369:HIS:HE1	2.04	0.41
1:B:272:SER:HB3	1:B:349:LYS:NZ	2.36	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	338/373 (91%)	331 (98%)	7 (2%)	0	100	100
1	B	333/373 (89%)	326 (98%)	7 (2%)	0	100	100
All	All	671/746 (90%)	657 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	283/330 (86%)	271 (96%)	12 (4%)	25	36
1	B	263/330 (80%)	252 (96%)	11 (4%)	25	36
All	All	546/660 (83%)	523 (96%)	23 (4%)	25	36

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	42	MET
1	A	108	ARG
1	A	138	LYS
1	A	156	SER
1	A	172	ASN
1	A	177	THR
1	A	185	THR
1	A	272	SER
1	A	316	LYS
1	A	318	SER
1	A	338	VAL
1	B	42	MET
1	B	62	ASP
1	B	110	GLN
1	B	111	ASP
1	B	172	ASN
1	B	185	THR
1	B	269	LYS
1	B	275	ASN
1	B	285	ASN
1	B	308	VAL
1	B	338	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	369	HIS
1	B	45	ASN
1	B	110	GLN
1	B	275	ASN

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Mol	Chain	Res	Type
1	B	285	ASN
1	B	369	HIS

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](#)

Of 3 ligands modelled in this entry, 3 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.

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

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	344/373 (92%)	0.31	12 (3%) 47 50	32, 58, 106, 126	0
1	B	343/373 (91%)	0.70	16 (4%) 37 39	47, 74, 112, 124	0
All	All	687/746 (92%)	0.51	28 (4%) 42 44	32, 68, 109, 126	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	4.8
1	A	14	LYS	3.7
1	A	296	ILE	3.6
1	B	276	LEU	3.3
1	B	279	SER	3.2
1	A	15	TYR	3.1
1	A	373	VAL	3.0
1	A	43	ILE	2.8
1	A	288	PHE	2.8
1	B	216	TRP	2.8
1	A	203	ASN	2.8
1	B	13	LEU	2.7
1	A	30	GLY	2.6
1	B	31	CYS	2.6
1	B	284	HIS	2.6
1	A	20	ILE	2.5
1	B	71	GLU	2.4
1	B	142	LEU	2.3
1	B	278	LYS	2.2
1	A	280	LEU	2.2
1	B	27	ILE	2.1
1	B	105	ALA	2.1
1	B	171	ASN	2.1
1	B	206	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	87	ILE	2.0
1	B	128	LEU	2.0
1	B	244	TYR	2.0
1	A	304	GLY	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](#)

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(\AA^2)	Q<0.9
3	NA	A	402	1/1	0.81	0.30	71,71,71,71	0
3	NA	B	401	1/1	0.94	0.26	64,64,64,64	0
2	CL	A	401	1/1	0.97	0.05	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.