



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:56 am BST

PDB ID : 4S2U  
Title : Crystal structure of the Phosphorybosylpyrophosphate synthetase from E. Coli  
Authors : Timofeev, V.I.; Abramchik, Y.A.; Muravieva, T.I.; Iaroslavtceva, A.K.; Stepanenko, V.N.; Zhukhlistova, N.E.; Esipov, R.S.; Kuranova, I.P.  
Deposited on : 2015-01-23  
Resolution : 2.71 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](mailto: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.

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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 : 2.11  
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) : 2.11

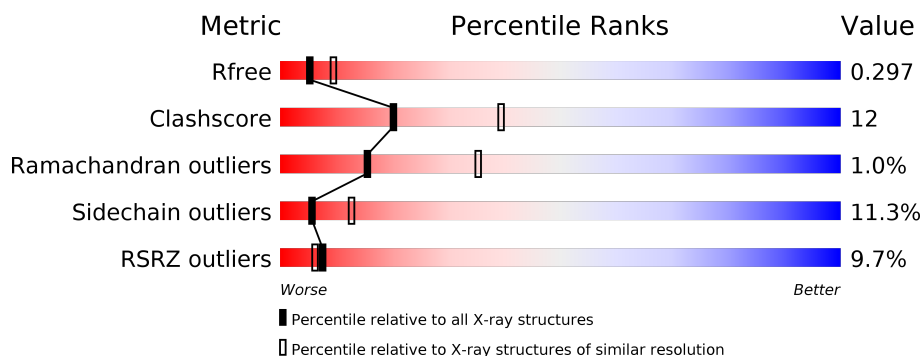
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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))
$R_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	316	<div> <div>9%</div> <div>70%</div> <div>24%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2351 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 Ribose-phosphate pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2339	1458	422	447	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP G4PTS0
A	1	ALA	-	EXPRESSION TAG	UNP G4PTS0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

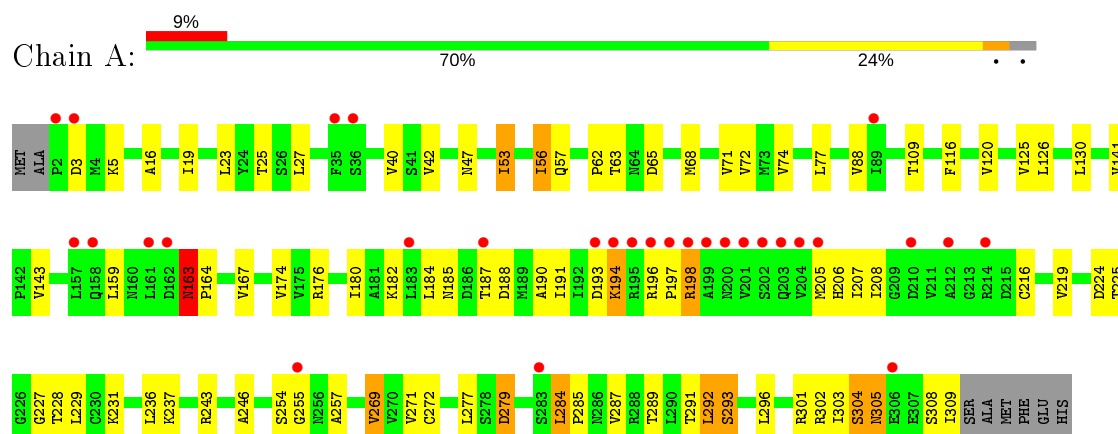
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Ribose-phosphate pyrophosphokinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.60 Å   104.60 Å   125.78 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	29.36 – 2.71 29.36 – 2.71	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.36-2.71) 94.6 (29.36-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.01 (at 2.72 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.250   ,   0.304 0.253   ,   0.297	Depositor DCC
$R_{free}$ test set	521 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.8	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2351	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: MG

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	0.42	0/2368	0.72	1/3213 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	163	ASN	C-N-CD	-5.41	108.70	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	SER	Peptide

### 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	2339	0	2381	59	0
2	A	1	0	0	0	0
3	A	11	0	0	0	0
All	All	2351	0	2381	59	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 12.

All (59) 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:224:ASP:OD1	1:A:254:SER:OG	2.08	0.70
1:A:187:THR:HB	1:A:188:ASP:CB	2.22	0.70
1:A:197:PRO:HB2	1:A:198:ARG:HB3	1.74	0.70
1:A:71:VAL:HG11	1:A:116:PHE:CZ	2.27	0.69
1:A:163:ASN:HB3	1:A:164:PRO:HA	1.74	0.68
1:A:174:VAL:HG22	1:A:191:ILE:HD12	1.78	0.66
1:A:193:ASP:HA	1:A:194:LYS:HB3	1.79	0.64
1:A:187:THR:HB	1:A:188:ASP:CG	2.18	0.64
1:A:277:LEU:HD11	1:A:289:THR:CG2	2.29	0.63
1:A:304:SER:N	1:A:305:ASN:HA	2.14	0.62
1:A:191:ILE:HG12	1:A:208:ILE:HD11	1.82	0.62
1:A:269:VAL:HG13	1:A:287:VAL:HG12	1.82	0.62
1:A:56:ILE:HD12	1:A:57:GLN:N	2.15	0.61
1:A:224:ASP:C	1:A:225:THR:HG23	2.21	0.61
1:A:19:ILE:HD11	1:A:56:ILE:HG21	1.84	0.60
1:A:225:THR:O	1:A:257:ALA:HA	2.01	0.59
1:A:180:ILE:HD13	1:A:219:VAL:HG21	1.86	0.58
1:A:190:ALA:O	1:A:191:ILE:HD13	2.04	0.57
1:A:56:ILE:C	1:A:56:ILE:HD12	2.27	0.56
1:A:53:ILE:CD1	1:A:77:LEU:HD13	2.38	0.54
1:A:301:ARG:O	1:A:304:SER:HB2	2.08	0.54
1:A:301:ARG:O	1:A:304:SER:N	2.41	0.54
1:A:304:SER:H	1:A:305:ASN:HA	1.73	0.53
1:A:277:LEU:HD11	1:A:289:THR:HG21	1.91	0.53
1:A:194:LYS:O	1:A:194:LYS:HD2	2.08	0.53
1:A:197:PRO:HB2	1:A:198:ARG:CB	2.39	0.52
1:A:74:VAL:HG11	1:A:120:VAL:HG13	1.92	0.51
1:A:284:LEU:HD23	1:A:285:PRO:HD2	1.93	0.50
1:A:125:VAL:CG2	1:A:143:VAL:HG13	2.42	0.49
1:A:16:ALA:O	1:A:19:ILE:HG12	2.13	0.49
1:A:271:VAL:O	1:A:289:THR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:HA	1:A:194:LYS:CB	2.44	0.48
1:A:302:ARG:O	1:A:305:ASN:HA	2.15	0.47
1:A:302:ARG:C	1:A:304:SER:H	2.18	0.47
1:A:125:VAL:HG22	1:A:143:VAL:HG22	1.97	0.47
1:A:167:VAL:HG13	1:A:190:ALA:HB3	1.96	0.46
1:A:68:MET:O	1:A:72:VAL:HG13	2.15	0.46
1:A:224:ASP:O	1:A:225:THR:OG1	2.30	0.46
1:A:62:PRO:HB2	1:A:65:ASP:HB2	1.97	0.46
1:A:74:VAL:CG1	1:A:120:VAL:HG13	2.47	0.45
1:A:180:ILE:CD1	1:A:219:VAL:HG21	2.47	0.45
1:A:53:ILE:HD11	1:A:77:LEU:HD13	1.98	0.45
1:A:309:ILE:O	1:A:309:ILE:HD12	2.16	0.45
1:A:187:THR:HB	1:A:188:ASP:CA	2.48	0.44
1:A:182:LYS:O	1:A:184:LEU:O	2.36	0.44
1:A:272:CYS:HB3	1:A:292:LEU:HD22	1.99	0.44
1:A:23:LEU:O	1:A:25:THR:HG23	2.18	0.43
1:A:197:PRO:HB2	1:A:198:ARG:CA	2.49	0.43
1:A:42:VAL:HG21	1:A:72:VAL:HG23	2.00	0.43
1:A:279:ASP:N	1:A:279:ASP:OD1	2.52	0.43
1:A:207:ILE:HG22	1:A:208:ILE:N	2.34	0.42
1:A:291:THR:HB	1:A:293:SER:OG	2.20	0.42
1:A:185:ASN:HD22	1:A:185:ASN:N	2.18	0.42
1:A:194:LYS:O	1:A:194:LYS:CG	2.68	0.42
1:A:216:CYS:SG	1:A:236:LEU:HD22	2.60	0.41
1:A:229:LEU:HD23	1:A:246:ALA:HB1	2.01	0.41
1:A:5:LYS:NZ	1:A:47:ASN:O	2.54	0.41
1:A:227:GLY:O	1:A:231:LYS:HD3	2.20	0.41
1:A:125:VAL:HG22	1:A:143:VAL:HG13	2.04	0.40

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	306/316 (97%)	269 (88%)	34 (11%)	3 (1%)	15	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	255	GLY
1	A	303	ILE

### 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	256/262 (98%)	227 (89%)	29 (11%)	6	13

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	27	LEU
1	A	40	VAL
1	A	53	ILE
1	A	56	ILE
1	A	63	THR
1	A	88	VAL
1	A	109	THR
1	A	126	LEU
1	A	130	LEU
1	A	141	VAL
1	A	159	LEU
1	A	176	ARG
1	A	194	LYS
1	A	196	ARG
1	A	198	ARG
1	A	205	MET
1	A	206	HIS

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Mol	Chain	Res	Type
1	A	228	THR
1	A	237	LYS
1	A	243	ARG
1	A	269	VAL
1	A	279	ASP
1	A	284	LEU
1	A	292	LEU
1	A	293	SER
1	A	296	LEU
1	A	305	ASN
1	A	308	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	21	ASN
1	A	64	ASN
1	A	163	ASN
1	A	185	ASN
1	A	256	ASN
1	A	259	ASN
1	A	263	ASN
1	A	305	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	308/316 (97%)	0.54	30 (9%) 7 6	23, 45, 102, 136	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	VAL	10.8
1	A	199	ALA	10.4
1	A	203	GLN	10.2
1	A	197	PRO	7.7
1	A	204	VAL	7.4
1	A	202	SER	6.6
1	A	200	ASN	5.6
1	A	198	ARG	5.0
1	A	187	THR	4.7
1	A	161	LEU	4.6
1	A	212	ALA	4.1
1	A	205	MET	3.8
1	A	196	ARG	3.7
1	A	193	ASP	3.6
1	A	162	ASP	3.5
1	A	36	SER	3.3
1	A	283	SER	3.2
1	A	195	ARG	3.2
1	A	183	LEU	3.0
1	A	210	ASP	2.9
1	A	214	ARG	2.9
1	A	2	PRO	2.8
1	A	158	GLN	2.7
1	A	306	GLU	2.7
1	A	194	LYS	2.4
1	A	89	ILE	2.3
1	A	255	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	35	PHE	2.1
1	A	3	ASP	2.1
1	A	157	LEU	2.1

## 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 carbohydrates 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, 95<sup>th</sup> 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	MG	A	401	1/1	0.96	0.27	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.