



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:56 PM GMT

PDB ID : 4JYZ  
Title : Crystal structure of E. coli glutaminyl-tRNA synthetase bound to ATP and native tRNA(Gln) containing the cmnm5s2U34 anticodon wobble base  
Authors : Perona, J.J.; Rodriguez-Hernandez, A.  
Deposited on : 2013-04-01  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

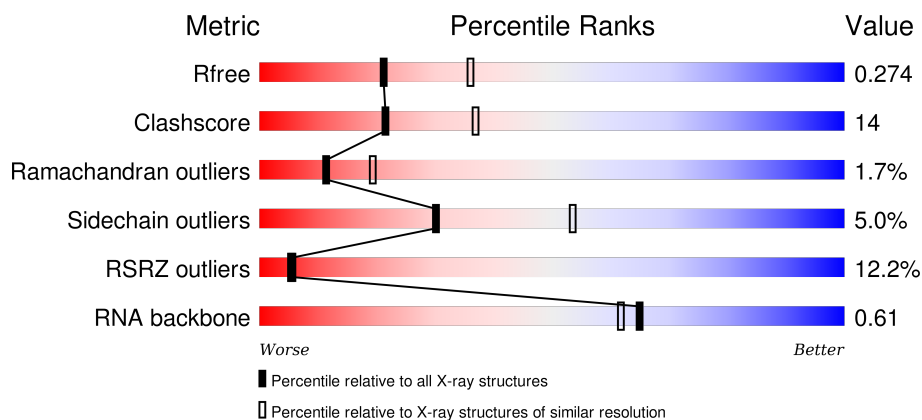
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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. 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	553	
2	B	75	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	603	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6022 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 Glutamine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4328	2737	764	806	21			

- Molecule 2 is a RNA chain called RNA (72-MER).

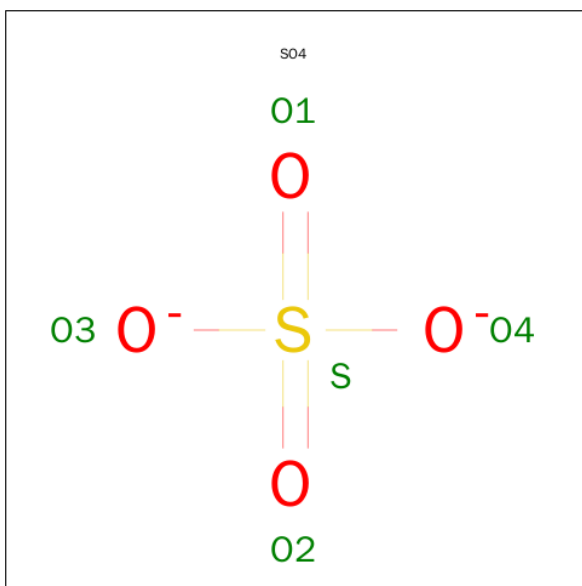
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	P	S	0	0
			1543	691	275	503	72	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

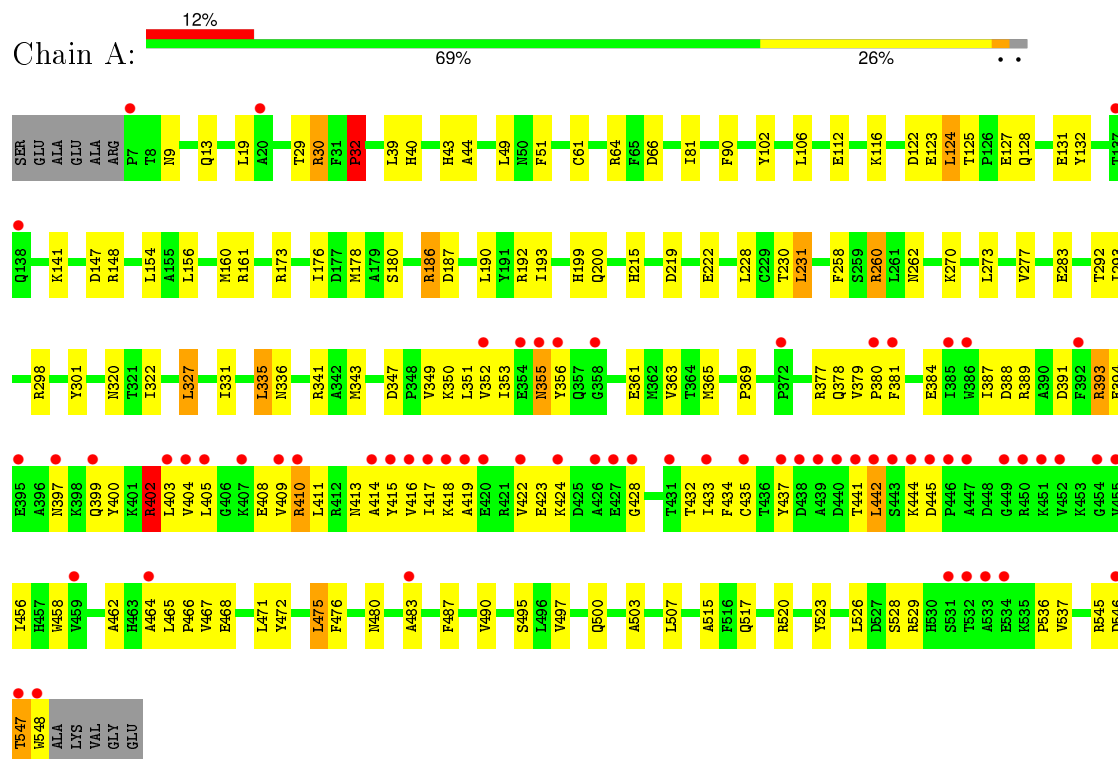
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	31	Total	O	0	0
			31	31		

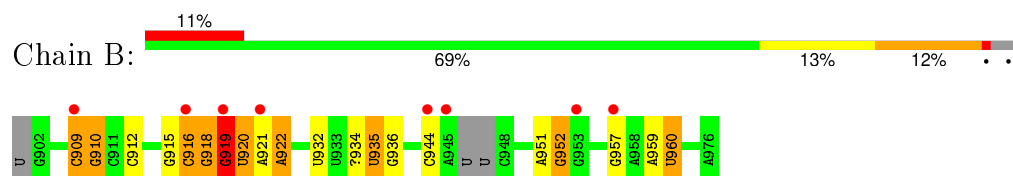
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Glutamine-tRNA ligase



#### • Molecule 2: RNA (72-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.40Å 234.62Å 113.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.50 47.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.60-2.50) 99.1 (47.55-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.234 , 0.263 0.241 , 0.274	Depositor DCC
$R_{free}$ test set	4269 reflections (9.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 82840 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 5MU, OMG, ATP, H2U, 1RN, 2MA, SO4, OMU, 4SU, PSU

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	0.39	0/4432	0.59	0/6009
2	B	0.44	0/1505	0.97	1/2340 (0.0%)
All	All	0.40	0/5937	0.72	1/8349 (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
2	B	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( $^{\circ}$ )
2	B	960	U	C2'-C3'-O3'	6.83	124.63	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	919	G	Sidechain

### 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	4328	0	4179	132	0
2	B	1543	0	791	24	0
3	A	31	0	12	2	0
4	A	10	0	0	0	0
5	A	79	0	0	4	0
5	B	31	0	0	1	0
All	All	6022	0	4982	151	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 14.

The worst 5 of 151 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)
2:B:919:G:H4'	2:B:920:H2U:OP1	1.53	1.04
1:A:503:ALA:HB1	1:A:507:LEU:HD12	1.57	0.84
1:A:39:LEU:HD13	1:A:81:ILE:HG12	1.61	0.81
1:A:403:LEU:HD13	1:A:409:VAL:HG12	1.63	0.80
1:A:397:ASN:ND2	1:A:399:GLN:HB2	2.00	0.77

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	540/553 (98%)	497 (92%)	34 (6%)	9 (2%)	<b>11</b> <b>19</b>

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	ALA
1	A	32	PRO
1	A	402	ARG
1	A	442	LEU
1	A	547	THR

### 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	458/481 (95%)	435 (95%)	23 (5%)	30 53

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	231	LEU
1	A	475	LEU
1	A	192	ARG
1	A	260	ARG

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

Mol	Chain	Res	Type
1	A	336	ASN
1	A	338	ASN
1	A	413	ASN
1	A	500	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	68/75 (90%)	10 (14%)	4 (5%)

5 of 10 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	909	C
2	B	910	G
2	B	916	C
2	B	918	OMG
2	B	919	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	909	C
2	B	919	G
2	B	935	U
2	B	960	U

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

9 non-standard protein/DNA/RNA residues 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	4SU	B	908	2	11,21,22	6.77	2 (18%)	13,30,33	2.71	1 (7%)
2	OMG	B	918	2	17,26,27	1.11	1 (5%)	21,38,41	3.32	5 (23%)
2	H2U	B	920	2	17,21,22	2.92	6 (35%)	23,30,33	7.25	11 (47%)
2	OMU	B	932	2	12,22,23	1.18	1 (8%)	19,31,34	3.28	3 (15%)
2	1RN	B	934	2	16,27,28	6.04	7 (43%)	17,38,41	3.20	5 (29%)
2	2MA	B	937	2	16,25,26	1.24	2 (12%)	18,37,40	1.97	1 (5%)
2	PSU	B	938	2	13,21,22	1.47	2 (15%)	18,30,33	3.48	4 (22%)
2	5MU	B	954	2	12,22,23	1.50	3 (25%)	14,32,35	4.66	2 (14%)
2	PSU	B	955	2	13,21,22	2.40	2 (15%)	18,30,33	3.81	5 (27%)

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	4SU	B	908	2	-	0/3/25/26	0/2/2/2
2	OMG	B	918	2	-	0/5/27/28	0/3/3/3
2	H2U	B	920	2	-	0/7/38/39	0/2/2/2
2	OMU	B	932	2	-	0/5/27/28	0/2/2/2
2	1RN	B	934	2	-	0/7/31/32	0/2/2/2
2	2MA	B	937	2	-	0/3/25/26	0/3/3/3
2	PSU	B	938	2	-	0/7/25/26	0/2/2/2
2	5MU	B	954	2	-	0/3/25/26	0/2/2/2
2	PSU	B	955	2	-	0/7/25/26	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	908	4SU	C4-S4	-21.87	1.25	1.67
2	B	934	1RN	C2-S2	-21.03	1.23	1.66
2	B	934	1RN	C7-N2	-9.11	1.23	1.47
2	B	955	PSU	C5-C1'	-7.86	1.45	1.52
2	B	920	H2U	C6-N1	-5.13	1.40	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	920	H2U	C4-N3-C2	-22.06	107.59	125.79
2	B	920	H2U	N3-C2-N1	-15.27	101.35	116.60
2	B	955	PSU	N1-C2-N3	-14.15	119.30	128.33
2	B	938	PSU	N1-C2-N3	-12.68	120.24	128.33
2	B	920	H2U	O2-C2-N3	-12.20	97.63	121.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	918	OMG	4	0
2	B	920	H2U	1	0
2	B	932	OMU	1	0
2	B	934	1RN	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 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	$\# Z  > 2$
3	ATP	A	601	-	24,33,33	1.64	4 (16%)	31,52,52	3.06	7 (22%)
4	SO4	A	602	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	A	603	-	4,4,4	0.27	0	6,6,6	0.07	0

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
3	ATP	A	601	-	-	0/18/38/38	0/3/3/3
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ATP	C5-C4	-2.96	1.33	1.40
3	A	601	ATP	O4'-C1'	2.42	1.44	1.41
3	A	601	ATP	C2-N1	3.38	1.40	1.33
3	A	601	ATP	C2-N3	4.51	1.40	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ATP	N3-C2-N1	-14.45	117.83	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ATP	PA-O3A-PB	-4.40	120.37	132.73
3	A	601	ATP	PB-O3B-PG	-4.07	119.02	132.67
3	A	601	ATP	C4'-O4'-C1'	-3.08	106.34	109.72
3	A	601	ATP	C4-C5-N7	-2.15	107.50	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ATP	2	0

## 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<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	542/553 (98%)	0.92	66 (12%) <b>5</b> <b>5</b>	27, 48, 90, 115	0
2	B	63/75 (84%)	0.85	8 (12%) <b>5</b> <b>5</b>	37, 71, 98, 112	0
All	All	605/628 (96%)	0.91	74 (12%) <b>5</b> <b>5</b>	27, 50, 92, 115	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	ALA	7.6
1	A	452	VAL	7.2
1	A	419	ALA	5.5
1	A	441	THR	5.5
1	A	450	ARG	5.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	2MA	B	937	23/24	0.95	0.16	-	64,70,71,72	0
2	OMU	B	932	21/22	0.87	0.22	-	89,93,95,97	0
2	PSU	B	955	20/21	0.81	0.28	-	84,98,105,105	0
2	PSU	B	938	20/21	0.95	0.17	-	66,71,84,85	0
2	1RN	B	934	26/27	0.86	0.27	-	86,97,114,115	0
2	H2U	B	920	20/21	0.92	0.28	-	89,91,93,93	0
2	5MU	B	954	21/22	0.81	0.25	-	87,97,100,104	0
2	OMG	B	918	24/25	0.85	0.26	-	81,90,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	4SU	B	908	20/21	0.82	0.24	-	64,78,104,123	0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	603	5/5	0.58	0.53	10.59	142,142,143,143	0
4	SO4	A	602	5/5	0.84	0.28	1.63	128,129,129,129	0
3	ATP	A	601	31/31	0.96	0.20	-0.49	36,41,68,69	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.