



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 AM GMT

PDB ID : 2TS1  
Title : STRUCTURE OF TYROSYL-T/RNA SYNTHETASE REFINED AT 2.3  
ANGSTROMS RESOLUTION. INTERACTION OF THE ENZYME WITH  
THE TYROSYL ADENYLATE INTERMEDIATE  
Authors : Brick, P.; Bhat, T.N.; Blow, D.M.  
Deposited on : 1989-06-29  
Resolution : 2.30 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  
<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

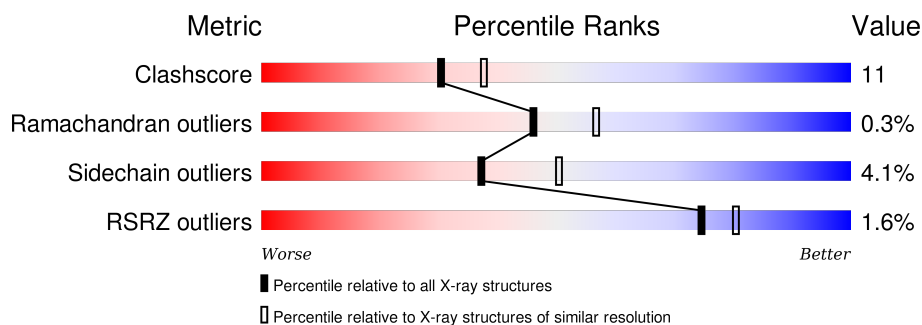
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 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	419	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2567 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 TYROSYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2457	1568	425	457	7			

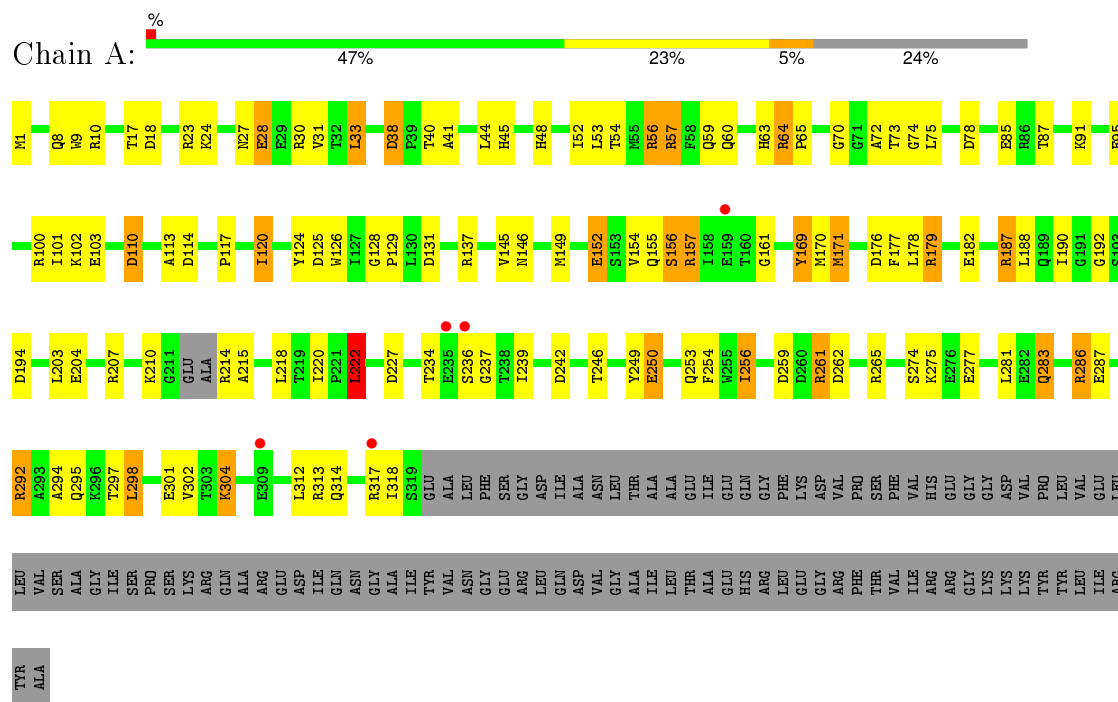
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		

### 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 ( $RSRZ > 2$ ). 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: TYROSYL-TRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.46 Å 64.46 Å 237.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30 45.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 97.5 (45.63-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.10 Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.228 , (Not available) 0.227 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 86.5	EDS
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 33905 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	2567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

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	1.05	1/2505 (0.0%)	2.02	76/3389 (2.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	GLU	CB-CG	-5.96	1.40	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH1	14.35	127.47	120.30
1	A	157	ARG	NE-CZ-NH2	-14.17	113.21	120.30
1	A	56	ARG	NE-CZ-NH2	-13.39	113.61	120.30
1	A	23	ARG	NE-CZ-NH2	-13.37	113.61	120.30
1	A	261	ARG	NE-CZ-NH1	12.01	126.30	120.30
1	A	157	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	179	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	23	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	261	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	A	292	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	64	ARG	CD-NE-CZ	10.35	138.10	123.60
1	A	110	ASP	CB-CG-OD1	10.33	127.59	118.30
1	A	10	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	A	137	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	A	313	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	A	137	ARG	CD-NE-CZ	8.96	136.14	123.60
1	A	179	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	A	41	ALA	N-CA-CB	8.45	121.92	110.10
1	A	286	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	169	TYR	CB-CG-CD1	-7.96	116.22	121.00
1	A	56	ARG	NH1-CZ-NH2	7.77	127.94	119.40
1	A	259	ASP	CB-CG-OD2	7.66	125.20	118.30
1	A	313	ARG	CD-NE-CZ	7.66	134.32	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ARG	CG-CD-NE	7.44	127.43	111.80
1	A	57	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	125	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	194	ASP	CB-CG-OD2	7.16	124.75	118.30
1	A	85	GLU	OE1-CD-OE2	7.15	131.88	123.30
1	A	28	GLU	CA-CB-CG	7.13	129.10	113.40
1	A	283	GLN	CB-CG-CD	7.03	129.89	111.60
1	A	38	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	A	227	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	171	MET	CA-CB-CG	6.61	124.54	113.30
1	A	298	LEU	CB-CG-CD2	-6.57	99.83	111.00
1	A	261	ARG	CD-NE-CZ	6.55	132.77	123.60
1	A	57	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	207	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	187	ARG	CD-NE-CZ	-6.41	114.63	123.60
1	A	157	ARG	N-CA-C	6.36	128.16	111.00
1	A	131	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	30	ARG	N-CA-CB	6.32	121.97	110.60
1	A	214	ARG	N-CA-CB	-6.24	99.37	110.60
1	A	317	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	126	TRP	CA-C-O	-5.94	107.62	120.10
1	A	87	THR	N-CA-CB	5.91	121.54	110.30
1	A	286	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	18	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	101	ILE	CB-CA-C	5.82	123.24	111.60
1	A	182	GLU	OE1-CD-OE2	-5.79	116.36	123.30
1	A	283	GLN	CB-CA-C	5.77	121.94	110.40
1	A	249	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	A	126	TRP	CB-CG-CD1	5.63	134.33	127.00
1	A	182	GLU	CG-CD-OE1	5.61	129.52	118.30
1	A	179	ARG	CD-NE-CZ	5.53	131.35	123.60
1	A	262	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	265	ARG	CA-CB-CG	5.43	125.35	113.40
1	A	204	GLU	CG-CD-OE1	5.40	129.11	118.30
1	A	103	GLU	CA-C-O	-5.40	108.77	120.10
1	A	110	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	250	GLU	CA-CB-CG	5.36	125.18	113.40
1	A	317	ARG	CG-CD-NE	-5.35	100.56	111.80
1	A	222	LEU	CB-CA-C	5.33	120.33	110.20
1	A	237	GLY	N-CA-C	-5.32	99.80	113.10
1	A	176	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	215	ALA	CB-CA-C	5.30	118.05	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	PHE	CB-CG-CD1	-5.28	117.11	120.80
1	A	194	ASP	O-C-N	5.24	131.08	122.70
1	A	126	TRP	O-C-N	5.22	131.06	122.70
1	A	313	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	28	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	A	40	THR	CA-CB-OG1	-5.16	98.16	109.00
1	A	120	ILE	N-CA-CB	5.16	122.66	110.80
1	A	192	GLY	C-N-CA	5.14	134.54	121.70
1	A	152	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	74	GLY	O-C-N	-5.09	114.56	122.70
1	A	157	ARG	CB-CA-C	-5.03	100.34	110.40

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	2457	0	2385	53	0
2	A	110	0	0	4	0
All	All	2567	0	2385	53	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 11.

All (53) 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:45:HIS:H	1:A:48:HIS:HD2	1.17	0.88
1:A:234:THR:HG22	1:A:236:SER:H	1.47	0.79
1:A:45:HIS:H	1:A:48:HIS:CD2	2.06	0.70
1:A:283:GLN:HG3	1:A:286:ARG:NH1	2.12	0.64
1:A:222:LEU:HD23	2:A:493:HOH:O	1.97	0.64
1:A:72:ALA:O	1:A:75:LEU:HB2	1.98	0.63
1:A:292:ARG:NH1	1:A:295:GLN:HG2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:O	1:A:149:MET:HG2	2.00	0.61
1:A:54:THR:HG21	1:A:220:ILE:HD11	1.81	0.61
1:A:48:HIS:O	1:A:52:ILE:HG13	2.00	0.60
1:A:100:ARG:NH2	1:A:242:ASP:OD1	2.32	0.60
1:A:31:VAL:O	1:A:63:HIS:HB3	2.00	0.60
1:A:253:GLN:HA	1:A:256:ILE:HG22	1.83	0.60
1:A:110:ASP:OD2	1:A:113:ALA:HB2	2.01	0.60
1:A:24:LYS:NZ	1:A:28:GLU:OE2	2.35	0.59
1:A:64:ARG:HD2	2:A:485:HOH:O	2.04	0.57
1:A:292:ARG:HH11	1:A:295:GLN:HG2	1.71	0.56
1:A:314:GLN:O	1:A:318:ILE:HG13	2.06	0.55
1:A:152:GLU:O	1:A:156:SER:HB2	2.07	0.55
1:A:157:ARG:O	1:A:161:GLY:N	2.39	0.54
1:A:33:LEU:HA	1:A:188:LEU:O	2.08	0.53
1:A:239:ILE:HG23	1:A:246:THR:HG21	1.91	0.53
1:A:9:TRP:CZ2	1:A:275:LYS:HG3	2.43	0.53
1:A:297:THR:O	1:A:301:GLU:HG2	2.09	0.53
1:A:178:LEU:HD11	1:A:210:LYS:HE2	1.90	0.53
1:A:256:ILE:O	1:A:292:ARG:NH1	2.42	0.53
1:A:234:THR:HG22	1:A:236:SER:N	2.19	0.53
1:A:75:LEU:HD21	1:A:91:LYS:HA	1.92	0.52
1:A:91:LYS:O	1:A:95:GLU:HB2	2.11	0.50
1:A:281:LEU:HD22	1:A:294:ALA:HA	1.94	0.50
1:A:73:THR:HB	1:A:169:TYR:CE1	2.48	0.49
1:A:59:GLN:HB2	1:A:65:PRO:HG3	1.95	0.49
1:A:274:SER:N	1:A:277:GLU:OE2	2.23	0.49
1:A:53:LEU:O	1:A:56:ARG:HB3	2.15	0.47
1:A:56:ARG:O	1:A:60:GLN:HG3	2.15	0.47
1:A:154:VAL:O	1:A:155:GLN:C	2.53	0.47
1:A:1:MET:N	1:A:27:ASN:HD21	2.12	0.47
1:A:53:LEU:O	1:A:57:ARG:HG3	2.15	0.46
1:A:78:ASP:HB2	1:A:169:TYR:CZ	2.51	0.46
1:A:17:THR:HG21	1:A:203:LEU:CD1	2.46	0.45
1:A:102:LYS:HG3	1:A:120:ILE:HG21	1.98	0.45
1:A:44:LEU:HD13	1:A:52:ILE:HD11	1.98	0.45
1:A:170:MET:HG3	1:A:171:MET:HE2	1.99	0.45
1:A:190:ILE:HA	1:A:218:LEU:O	2.17	0.44
1:A:187:ARG:HG3	2:A:420:HOH:O	2.18	0.44
1:A:72:ALA:HB2	1:A:124:TYR:HA	2.01	0.43
1:A:298:LEU:O	1:A:302:VAL:HG23	2.19	0.43
1:A:38:ASP:OD2	1:A:70:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TRP:CH2	1:A:275:LYS:HA	2.55	0.42
1:A:304:LYS:HG3	1:A:312:LEU:HD22	2.02	0.42
1:A:250:GLU:HG2	2:A:525:HOH:O	2.20	0.41
1:A:113:ALA:O	1:A:117:PRO:HB3	2.22	0.40
1:A:128:GLY:N	1:A:129:PRO:HD2	2.37	0.40

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	313/419 (75%)	304 (97%)	8 (3%)	1 (0%)	46 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	SER

### 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	Percentiles
1	A	244/349 (70%)	234 (96%)	10 (4%)	37 50

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	33	LEU
1	A	114	ASP
1	A	146	ASN
1	A	177	PHE
1	A	179	ARG
1	A	222	LEU
1	A	256	ILE
1	A	261	ARG
1	A	304	LYS

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

Mol	Chain	Res	Type
1	A	27	ASN
1	A	48	HIS
1	A	60	GLN
1	A	89	ASN
1	A	155	GLN
1	A	283	GLN
1	A	314	GLN

### 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 ⓘ

There are no ligands in this entry.

## 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 [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	317/419 (75%)	-0.34	5 (1%) 74 80	2, 13, 33, 48	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	SER	3.5
1	A	317	ARG	2.7
1	A	309	GLU	2.7
1	A	159	GLU	2.4
1	A	235	GLU	2.3

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.