



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:37 am GMT

PDB ID : 3PRH  
Title : tryptophanyl-tRNA synthetase Val144Pro mutant from *B. subtilis*  
Authors : Antonczak, A.K.; Simova, Z.; Yonemoto, I.; Bochtler, M.; Piasecka, A.; Czapinska, H.; Brancale, A.; Tippmann, E.M.  
Deposited on : 2010-11-29  
Resolution : 2.80 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

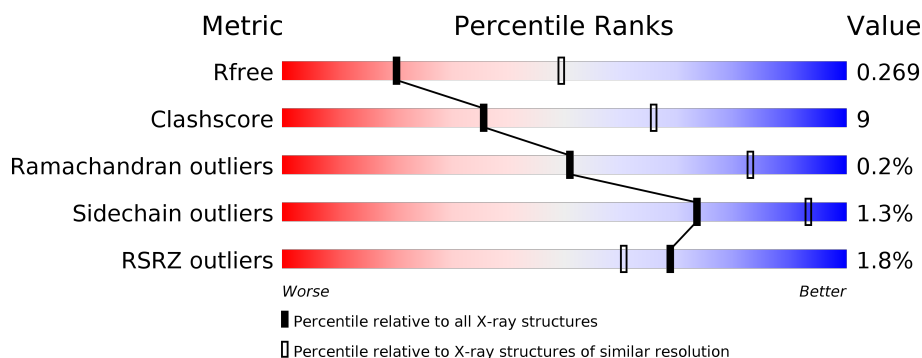
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	388	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>15%</div> <div>19%</div> </div> </div>
1	B	388	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>19%</div> <div>•</div> <div>20%</div> </div> </div>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4956 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2490	1583	418	477	12			
1	B	309	Total	C	N	O	S	0	2	0
			2466	1568	414	472	12			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	EXPRESSION TAG	UNP P21656
A	-31	HIS	-	EXPRESSION TAG	UNP P21656
A	-30	HIS	-	EXPRESSION TAG	UNP P21656
A	-29	HIS	-	EXPRESSION TAG	UNP P21656
A	-28	HIS	-	EXPRESSION TAG	UNP P21656
A	-27	HIS	-	EXPRESSION TAG	UNP P21656
A	-26	HIS	-	EXPRESSION TAG	UNP P21656
A	-25	GLY	-	EXPRESSION TAG	UNP P21656
A	-24	LYS	-	EXPRESSION TAG	UNP P21656
A	-23	PRO	-	EXPRESSION TAG	UNP P21656
A	-22	ILE	-	EXPRESSION TAG	UNP P21656
A	-21	PRO	-	EXPRESSION TAG	UNP P21656
A	-20	ASN	-	EXPRESSION TAG	UNP P21656
A	-19	PRO	-	EXPRESSION TAG	UNP P21656
A	-18	LEU	-	EXPRESSION TAG	UNP P21656
A	-17	LEU	-	EXPRESSION TAG	UNP P21656
A	-16	GLY	-	EXPRESSION TAG	UNP P21656
A	-15	LEU	-	EXPRESSION TAG	UNP P21656
A	-14	ASP	-	EXPRESSION TAG	UNP P21656
A	-13	SER	-	EXPRESSION TAG	UNP P21656
A	-12	THR	-	EXPRESSION TAG	UNP P21656
A	-11	GLU	-	EXPRESSION TAG	UNP P21656
A	-10	ASN	-	EXPRESSION TAG	UNP P21656
A	-9	LEU	-	EXPRESSION TAG	UNP P21656
A	-8	TYR	-	EXPRESSION TAG	UNP P21656

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	PHE	-	EXPRESSION TAG	UNP P21656
A	-6	GLN	-	EXPRESSION TAG	UNP P21656
A	-5	GLY	-	EXPRESSION TAG	UNP P21656
A	-4	ILE	-	EXPRESSION TAG	UNP P21656
A	-3	ASP	-	EXPRESSION TAG	UNP P21656
A	-2	PRO	-	EXPRESSION TAG	UNP P21656
A	-1	PHE	-	EXPRESSION TAG	UNP P21656
A	0	THR	-	EXPRESSION TAG	UNP P21656
A	144	PRO	VAL	ENGINEERED MUTATION	UNP P21656
A	330	GLN	-	EXPRESSION TAG	UNP P21656
A	331	GLY	-	EXPRESSION TAG	UNP P21656
A	332	ARG	-	EXPRESSION TAG	UNP P21656
A	333	ALA	-	EXPRESSION TAG	UNP P21656
A	334	GLN	-	EXPRESSION TAG	UNP P21656
A	335	ILE	-	EXPRESSION TAG	UNP P21656
A	336	ARG	-	EXPRESSION TAG	UNP P21656
A	337	LEU	-	EXPRESSION TAG	UNP P21656
A	338	LEU	-	EXPRESSION TAG	UNP P21656
A	339	THR	-	EXPRESSION TAG	UNP P21656
A	340	LYS	-	EXPRESSION TAG	UNP P21656
A	341	PRO	-	EXPRESSION TAG	UNP P21656
A	342	GLU	-	EXPRESSION TAG	UNP P21656
A	343	ARG	-	EXPRESSION TAG	UNP P21656
A	344	LYS	-	EXPRESSION TAG	UNP P21656
A	345	LEU	-	EXPRESSION TAG	UNP P21656
A	346	SER	-	EXPRESSION TAG	UNP P21656
A	347	TRP	-	EXPRESSION TAG	UNP P21656
A	348	LEU	-	EXPRESSION TAG	UNP P21656
A	349	LEU	-	EXPRESSION TAG	UNP P21656
A	350	PRO	-	EXPRESSION TAG	UNP P21656
A	351	PRO	-	EXPRESSION TAG	UNP P21656
A	352	LEU	-	EXPRESSION TAG	UNP P21656
A	353	SER	-	EXPRESSION TAG	UNP P21656
A	354	ASN	-	EXPRESSION TAG	UNP P21656
A	355	ASN	-	EXPRESSION TAG	UNP P21656
B	-32	MET	-	EXPRESSION TAG	UNP P21656
B	-31	HIS	-	EXPRESSION TAG	UNP P21656
B	-30	HIS	-	EXPRESSION TAG	UNP P21656
B	-29	HIS	-	EXPRESSION TAG	UNP P21656
B	-28	HIS	-	EXPRESSION TAG	UNP P21656
B	-27	HIS	-	EXPRESSION TAG	UNP P21656
B	-26	HIS	-	EXPRESSION TAG	UNP P21656

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-25	GLY	-	EXPRESSION TAG	UNP P21656
B	-24	LYS	-	EXPRESSION TAG	UNP P21656
B	-23	PRO	-	EXPRESSION TAG	UNP P21656
B	-22	ILE	-	EXPRESSION TAG	UNP P21656
B	-21	PRO	-	EXPRESSION TAG	UNP P21656
B	-20	ASN	-	EXPRESSION TAG	UNP P21656
B	-19	PRO	-	EXPRESSION TAG	UNP P21656
B	-18	LEU	-	EXPRESSION TAG	UNP P21656
B	-17	LEU	-	EXPRESSION TAG	UNP P21656
B	-16	GLY	-	EXPRESSION TAG	UNP P21656
B	-15	LEU	-	EXPRESSION TAG	UNP P21656
B	-14	ASP	-	EXPRESSION TAG	UNP P21656
B	-13	SER	-	EXPRESSION TAG	UNP P21656
B	-12	THR	-	EXPRESSION TAG	UNP P21656
B	-11	GLU	-	EXPRESSION TAG	UNP P21656
B	-10	ASN	-	EXPRESSION TAG	UNP P21656
B	-9	LEU	-	EXPRESSION TAG	UNP P21656
B	-8	TYR	-	EXPRESSION TAG	UNP P21656
B	-7	PHE	-	EXPRESSION TAG	UNP P21656
B	-6	GLN	-	EXPRESSION TAG	UNP P21656
B	-5	GLY	-	EXPRESSION TAG	UNP P21656
B	-4	ILE	-	EXPRESSION TAG	UNP P21656
B	-3	ASP	-	EXPRESSION TAG	UNP P21656
B	-2	PRO	-	EXPRESSION TAG	UNP P21656
B	-1	PHE	-	EXPRESSION TAG	UNP P21656
B	0	THR	-	EXPRESSION TAG	UNP P21656
B	144	PRO	VAL	ENGINEERED MUTATION	UNP P21656
B	330	GLN	-	EXPRESSION TAG	UNP P21656
B	331	GLY	-	EXPRESSION TAG	UNP P21656
B	332	ARG	-	EXPRESSION TAG	UNP P21656
B	333	ALA	-	EXPRESSION TAG	UNP P21656
B	334	GLN	-	EXPRESSION TAG	UNP P21656
B	335	ILE	-	EXPRESSION TAG	UNP P21656
B	336	ARG	-	EXPRESSION TAG	UNP P21656
B	337	LEU	-	EXPRESSION TAG	UNP P21656
B	338	LEU	-	EXPRESSION TAG	UNP P21656
B	339	THR	-	EXPRESSION TAG	UNP P21656
B	340	LYS	-	EXPRESSION TAG	UNP P21656
B	341	PRO	-	EXPRESSION TAG	UNP P21656
B	342	GLU	-	EXPRESSION TAG	UNP P21656
B	343	ARG	-	EXPRESSION TAG	UNP P21656
B	344	LYS	-	EXPRESSION TAG	UNP P21656

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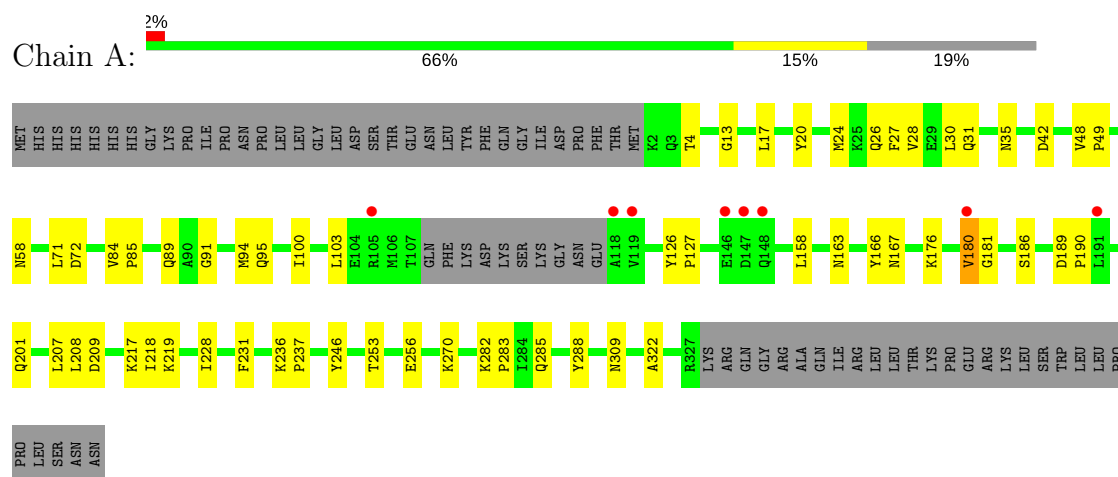
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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	LEU	-	EXPRESSION TAG	UNP P21656
B	346	SER	-	EXPRESSION TAG	UNP P21656
B	347	TRP	-	EXPRESSION TAG	UNP P21656
B	348	LEU	-	EXPRESSION TAG	UNP P21656
B	349	LEU	-	EXPRESSION TAG	UNP P21656
B	350	PRO	-	EXPRESSION TAG	UNP P21656
B	351	PRO	-	EXPRESSION TAG	UNP P21656
B	352	LEU	-	EXPRESSION TAG	UNP P21656
B	353	SER	-	EXPRESSION TAG	UNP P21656
B	354	ASN	-	EXPRESSION TAG	UNP P21656
B	355	ASN	-	EXPRESSION TAG	UNP P21656

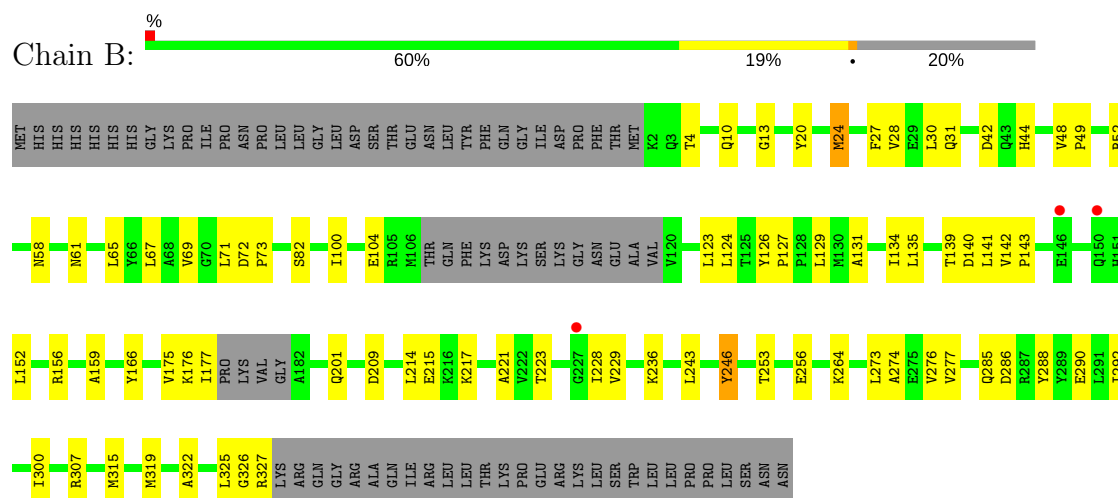
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Tryptophanyl-tRNA synthetase



#### • Molecule 1: Tryptophanyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.26Å 119.82Å 127.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.80 29.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.95-2.80) 100.0 (29.09-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.40 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.235 , 0.275 0.235 , 0.269	Depositor DCC
$R_{free}$ test set	913 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

### 5.1 Standard geometry

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	0.57	0/2531	0.65	0/3415
1	B	0.60	0/2507	0.66	0/3381
All	All	0.58	0/5038	0.66	0/6796

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	2490	0	2531	38	0
1	B	2466	0	2492	56	0
All	All	4956	0	5023	92	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 9.

The worst 5 of 92 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:B:24:MET:O	1:B:28:VAL:HG23	1.88	0.74
1:A:253:THR:OG1	1:A:256:GLU:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:OE1	1:A:72:ASP:N	2.24	0.68
1:B:175:VAL:HG13	1:B:175:VAL:O	1.99	0.63
1:A:228:ILE:O	1:A:236:LYS:NZ	2.31	0.63

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	312/388 (80%)	292 (94%)	19 (6%)	1 (0%)	44	77
1	B	305/388 (79%)	284 (93%)	21 (7%)	0	100	100
All	All	617/776 (80%)	576 (93%)	40 (6%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL

### 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	271/337 (80%)	269 (99%)	2 (1%)	87	97
1	B	268/337 (80%)	263 (98%)	5 (2%)	62	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	539/674 (80%)	532 (99%)	7 (1%)	73 93

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	MET
1	B	264	LYS
1	B	52	ARG
1	A	246	TYR
1	B	246	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	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 carbohydrates 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 ⓘ

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	316/388 (81%)	-0.03	8 (2%) 58 47	31, 53, 75, 85	0
1	B	309/388 (79%)	-0.13	3 (0%) 82 77	32, 53, 75, 84	0
All	All	625/776 (80%)	-0.08	11 (1%) 69 60	31, 53, 75, 85	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ARG	3.2
1	A	146	GLU	3.0
1	A	180	VAL	3.0
1	A	119	VAL	2.8
1	A	118	ALA	2.8

### 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.