



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2017 – 05:15 PM EDT

PDB ID : 1GGM  
Title : GLYCYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS  
COMPLEXED WITH GLYCYL-ADENYLATE  
Authors : Arnez, J.G.; Moras, D.  
Deposited on : unknown  
Resolution : 3.40 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
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) : rb-20030345

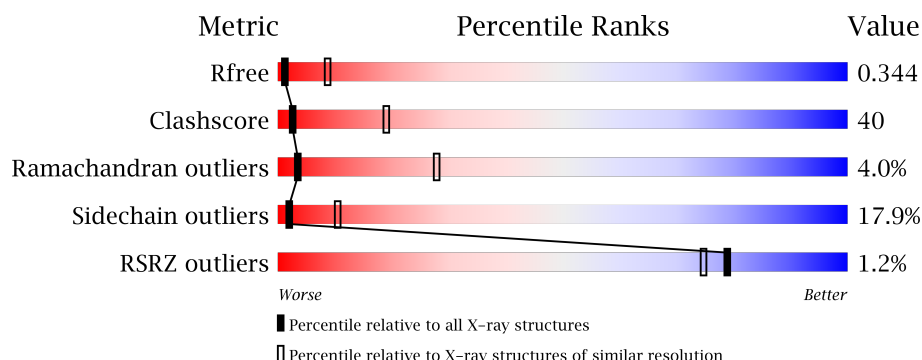
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	442	<div> <div>0.1%</div> <div>37% 50% 13%</div> </div>
1	B	442	<div> <div>2%</div> <div>39% 48% 13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8959 atoms, of which 1692 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 Glycine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	H	N	O	S	0	0	0
			4451	2297	841	649	656	8			
1	B	442	Total	C	H	N	O	S	0	0	0
			4440	2288	839	649	656	8			

There are 44 discrepancies between the modelled and reference sequences:

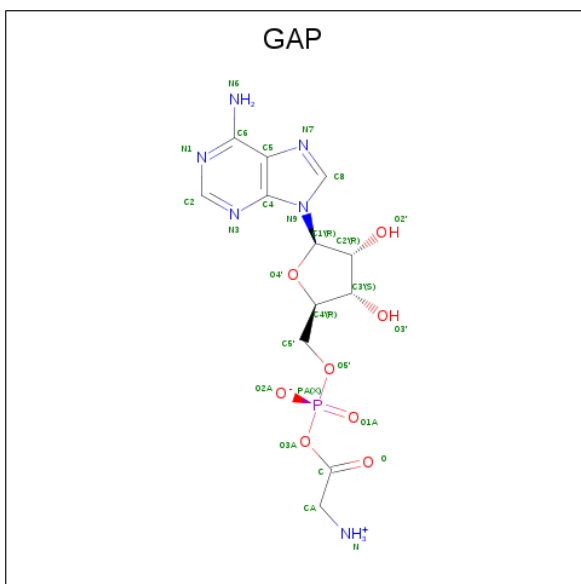
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	PRO	conflict	UNP P56206
A	91	ALA	ARG	conflict	UNP P56206
A	92	LYS	ILE	conflict	UNP P56206
A	93	ALA	THR	conflict	UNP P56206
A	94	ARG	LYS	conflict	UNP P56206
A	95	TYR	LYS	conflict	UNP P56206
A	170	GLN	LYS	conflict	UNP P56206
A	171	ASP	THR	conflict	UNP P56206
A	172	LEU	TYR	conflict	UNP P56206
A	173	ARG	VAL	conflict	UNP P56206
A	176	ARG	VAL	conflict	UNP P56206
A	177	GLY	GLU	conflict	UNP P56206
A	178	GLY	ASP	conflict	UNP P56206
A	179	ARG	GLU	conflict	UNP P56206
A	180	GLY	ALA	conflict	UNP P56206
A	181	LEU	SER	conflict	UNP P56206
A	209	GLY	PRO	conflict	UNP P56206
A	283	SER	GLU	conflict	UNP P56206
A	284	SER	LEU	conflict	UNP P56206
A	302	SER	LEU	conflict	UNP P56206
A	303	LEU	GLU	conflict	UNP P56206
A	310	GLN	ASN	conflict	UNP P56206
B	1	ALA	PRO	conflict	UNP P56206
B	91	ALA	ARG	conflict	UNP P56206
B	92	LYS	ILE	conflict	UNP P56206

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Chain	Residue	Modelled	Actual	Comment	Reference
B	93	ALA	THR	conflict	UNP P56206
B	94	ARG	LYS	conflict	UNP P56206
B	95	TYR	LYS	conflict	UNP P56206
B	170	GLN	LYS	conflict	UNP P56206
B	171	ASP	THR	conflict	UNP P56206
B	172	LEU	TYR	conflict	UNP P56206
B	173	ARG	VAL	conflict	UNP P56206
B	176	ARG	VAL	conflict	UNP P56206
B	177	GLY	GLU	conflict	UNP P56206
B	178	GLY	ASP	conflict	UNP P56206
B	179	ARG	GLU	conflict	UNP P56206
B	180	GLY	ALA	conflict	UNP P56206
B	181	LEU	SER	conflict	UNP P56206
B	209	GLY	PRO	conflict	UNP P56206
B	283	SER	GLU	conflict	UNP P56206
B	284	SER	LEU	conflict	UNP P56206
B	302	SER	LEU	conflict	UNP P56206
B	303	LEU	GLU	conflict	UNP P56206
B	310	GLN	ASN	conflict	UNP P56206

- Molecule 2 is GLYCYL-ADENOSINE-5'-PHOSPHATE (three-letter code: GAP) (formula:  $C_{12}H_{17}N_6O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			33	12	6	6	8	1	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			33	12	6	6	8	1		

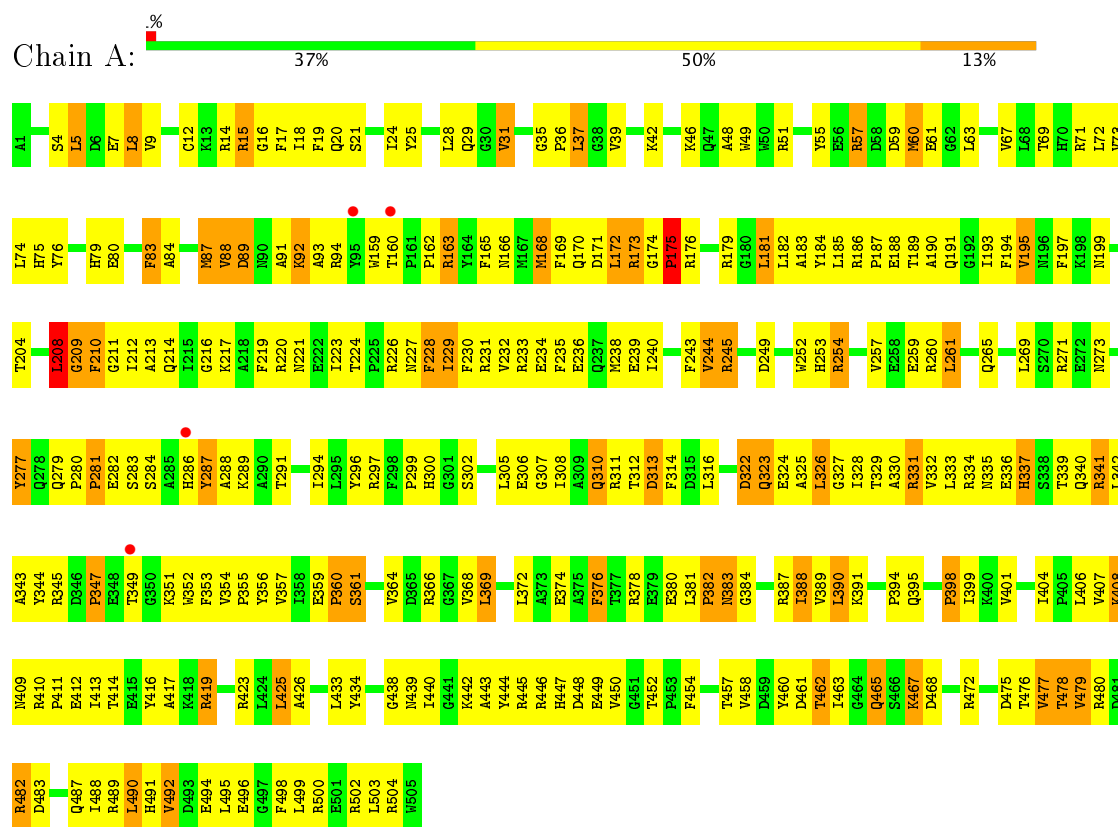
- Molecule 3 is water.

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

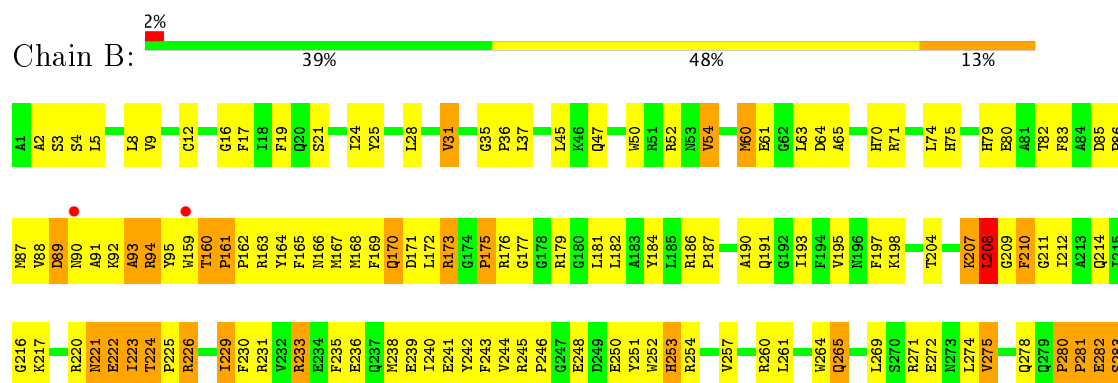
### 3 Residue-property plots

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: Glycine-tRNA ligase



#### • Molecule 1: Glycine-tRNA ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.50Å 250.10Å 106.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 3.40 11.99 – 3.39	Depositor EDS
% Data completeness (in resolution range)	89.0 (9.00-3.40) 90.3 (11.99-3.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	7.30	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.35Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.242 , 0.334 0.256 , 0.344	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 92.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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

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

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	0.72	1/3696 (0.0%)	0.95	5/4999 (0.1%)
1	B	0.67	0/3686	0.91	4/4986 (0.1%)
All	All	0.70	1/7382 (0.0%)	0.93	9/9985 (0.1%)

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
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	PHE	CB-CG	-5.30	1.42	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLY	C-N-CD	-10.13	98.30	120.60
1	B	208	LEU	N-CA-C	6.67	129.01	111.00
1	A	208	LEU	N-CA-C	6.24	127.84	111.00
1	A	59	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	224	THR	C-N-CD	-5.52	108.45	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	TYR	Sidechain
1	B	416	TYR	Sidechain

## 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	3610	841	3565	325	0
1	B	3601	839	3547	272	0
2	A	27	6	17	3	0
2	B	27	6	17	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7267	1692	7146	578	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 40.

The worst 5 of 578 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:366:ARG:NH1	2:A:1550:GAP:H2'	1.65	1.12
1:A:15:ARG:HH12	1:A:446:ARG:HA	1.23	1.03
1:B:310:GLN:NE2	1:B:312:THR:HG23	1.74	1.03
1:B:381:LEU:HD21	1:B:387:ARG:HD3	1.41	1.02
1:A:313:ASP:HB2	1:A:354:VAL:HG12	1.49	0.94

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	438/442 (99%)	359 (82%)	62 (14%)	17 (4%)	3	28
1	B	438/442 (99%)	351 (80%)	69 (16%)	18 (4%)	3	27
All	All	876/884 (99%)	710 (81%)	131 (15%)	35 (4%)	3	28

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PRO
1	A	228	PHE
1	B	89	ASP
1	B	93	ALA
1	B	175	PRO

### 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	375/376 (100%)	306 (82%)	69 (18%)	2	9
1	B	374/376 (100%)	309 (83%)	65 (17%)	2	12
All	All	749/752 (100%)	615 (82%)	134 (18%)	2	10

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	ASP
1	B	60	MET
1	B	442	LYS
1	A	477	VAL
1	A	504	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	GLN
1	A	323	GLN
1	B	265	GLN
1	A	278	GLN
1	B	214	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](#)

2 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	$\# Z  > 2$
2	GAP	A	1550	-	25,29,29	0.76	0	25,43,43	1.21	1 (4%)
2	GAP	B	2550	-	25,29,29	0.70	0	25,43,43	1.01	2 (8%)

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	GAP	A	1550	-	-	0/11/33/33	0/3/3/3
2	GAP	B	2550	-	-	0/11/33/33	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	2550	GAP	O-C-CA	-2.05	113.23	117.92
2	B	2550	GAP	O2A-PA-O3A	2.43	111.81	104.11
2	A	1550	GAP	C-CA-N	4.25	117.51	111.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1550	GAP	3	0
2	B	2550	GAP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance ( $\text{\AA}$ )
1	A	95:TYR	C	159:TRP	N	11.89
1	B	95:TYR	C	159:TRP	N	10.93

## 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	442/442 (100%)	-0.45	4 (0%) 84 80	12, 39, 77, 104	0
1	B	442/442 (100%)	-0.40	7 (1%) 72 67	12, 43, 84, 108	0
All	All	884/884 (100%)	-0.42	11 (1%) 79 75	12, 41, 81, 108	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	HIS	3.4
1	B	159	TRP	3.2
1	B	90	ASN	2.8
1	A	286	HIS	2.6
1	A	160	THR	2.5

### 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. 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
2	GAP	B	2550	27/27	0.94	0.20	0.66	0,46,58,61	0
2	GAP	A	1550	27/27	0.94	0.17	-0.09	0,28,42,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.