



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2017 – 10:58 AM EDT

PDB ID : 5IG5  
Title : Crystal structure of N. vectensis CaMKII-B hub at pH 4.2  
Authors : Bhattacharyya, M.; Gee, C.L.; Barros, T.; Kuriyan, J.  
Deposited on : unknown  
Resolution : 3.00 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	:	rb-20029824
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-20029824

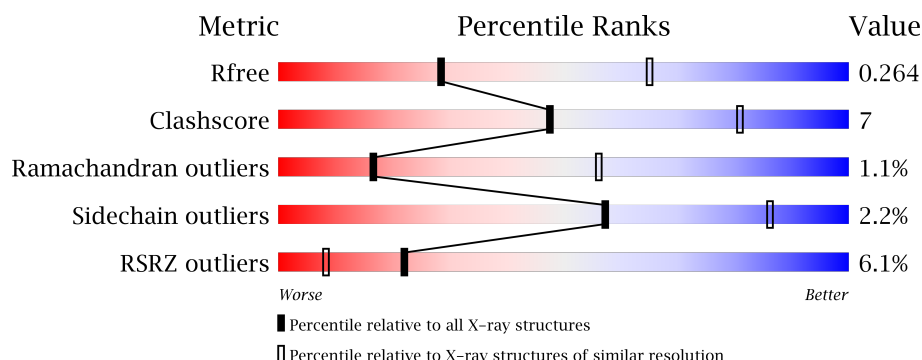
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	145	<div> <div>0.1%</div> <div>75%</div> <div>16%</div> <div>6%</div> </div>
1	B	145	<div> <div>5%</div> <div>74%</div> <div>18%</div> <div>5%</div> </div>
1	C	145	<div> <div>10%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
1	D	145	<div> <div>12%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	E	145	<div> <div>0.1%</div> <div>81%</div> <div>14%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	145	<div><div></div><div>5%</div><div></div><div>78%</div><div></div><div>19%</div><div></div><div>• •</div></div>
1	G	145	<div><div></div><div>6%</div><div></div><div>62%</div><div></div><div>32%</div><div></div><div>• 5%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8925 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 CaMKII-B hub.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1100	695	188	215	2			
1	F	143	Total	C	N	O	S	0	1	0
			1164	732	206	224	2			
1	C	137	Total	C	N	O	S	0	0	0
			1104	697	191	214	2			
1	D	136	Total	C	N	O	S	0	0	0
			1094	690	188	214	2			
1	E	139	Total	C	N	O	S	0	0	0
			1118	707	193	216	2			
1	B	138	Total	C	N	O	S	0	0	0
			1111	701	192	216	2			
1	G	138	Total	C	N	O	S	0	138	0
			2222	1402	384	432	4			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	GLY	-	expression tag	UNP A7RF52
A	331	PRO	-	expression tag	UNP A7RF52
A	332	HIS	-	expression tag	UNP A7RF52
B	330	GLY	-	expression tag	UNP A7RF52
B	331	PRO	-	expression tag	UNP A7RF52
B	332	HIS	-	expression tag	UNP A7RF52
C	330	GLY	-	expression tag	UNP A7RF52
C	331	PRO	-	expression tag	UNP A7RF52
C	332	HIS	-	expression tag	UNP A7RF52
D	330	GLY	-	expression tag	UNP A7RF52
D	331	PRO	-	expression tag	UNP A7RF52
D	332	HIS	-	expression tag	UNP A7RF52
E	330	GLY	-	expression tag	UNP A7RF52
E	331	PRO	-	expression tag	UNP A7RF52
E	332	HIS	-	expression tag	UNP A7RF52

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Chain	Residue	Modelled	Actual	Comment	Reference
F	330	GLY	-	expression tag	UNP A7RF52
F	331	PRO	-	expression tag	UNP A7RF52
F	332	HIS	-	expression tag	UNP A7RF52
G	330	GLY	-	expression tag	UNP A7RF52
G	331	PRO	-	expression tag	UNP A7RF52
G	332	HIS	-	expression tag	UNP A7RF52

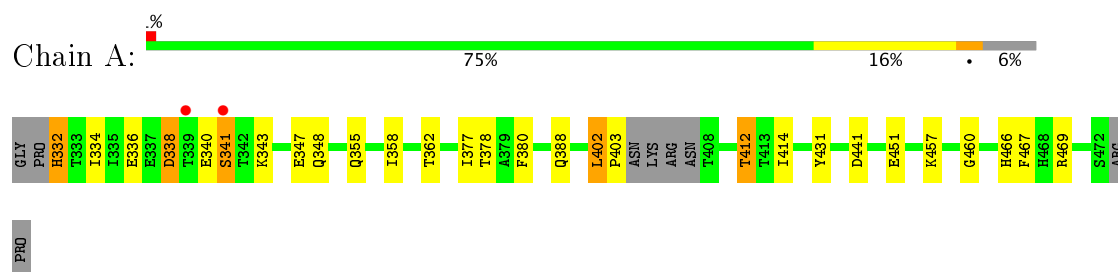
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	F	2	Total O 2 2	0	0
2	C	2	Total O 2 2	0	0
2	D	2	Total O 2 2	0	0
2	E	2	Total O 2 2	0	0
2	B	3	Total O 3 3	0	0

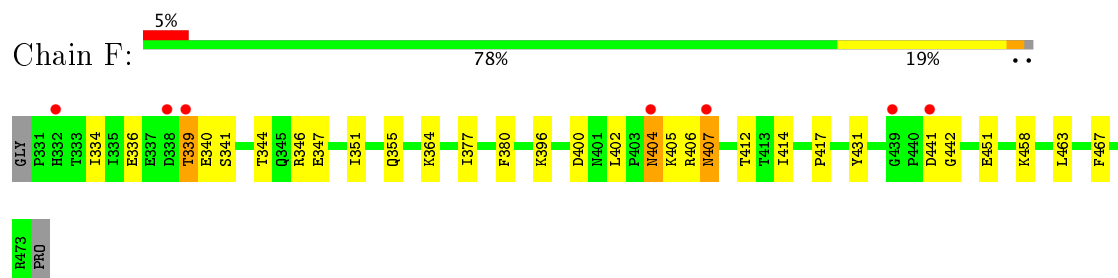
### 3 Residue-property plots [i](#)

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.

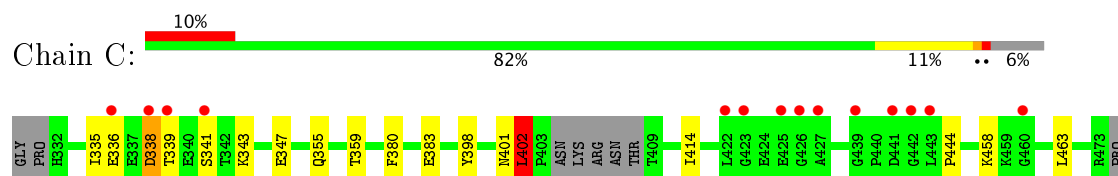
- Molecule 1: CaMKII-B hub



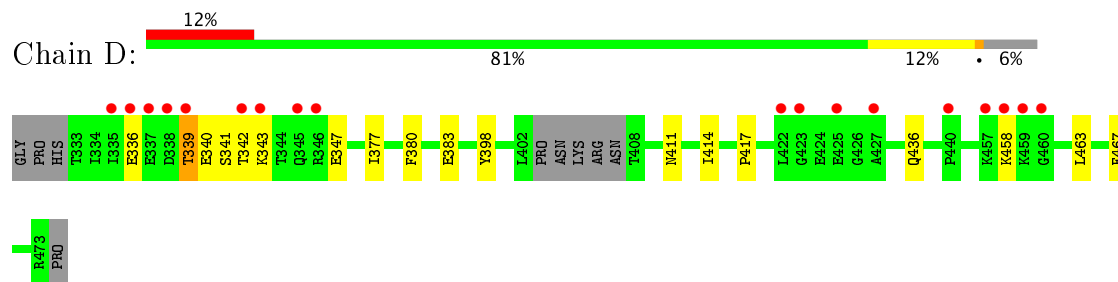
- Molecule 1: CaMKII-B hub



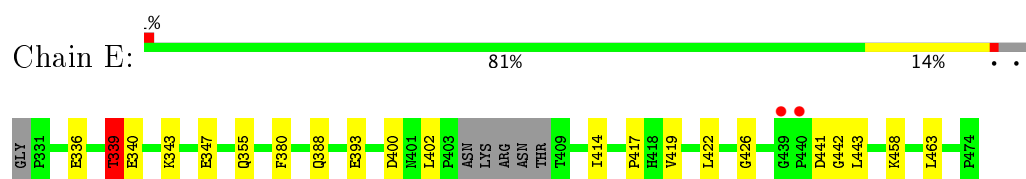
- Molecule 1: CaMKII-B hub



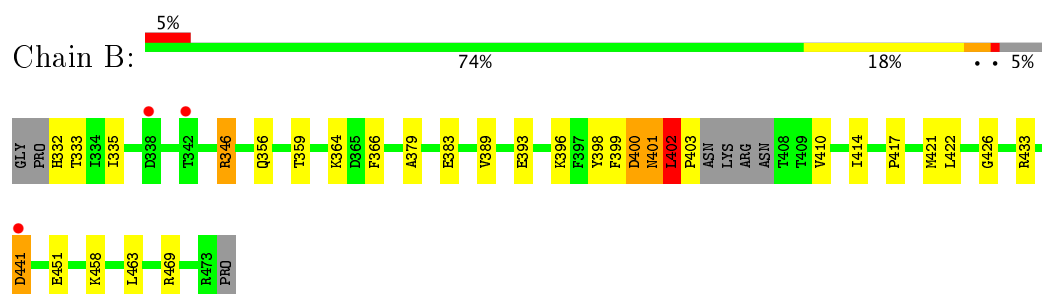
- Molecule 1: CaMKII-B hub



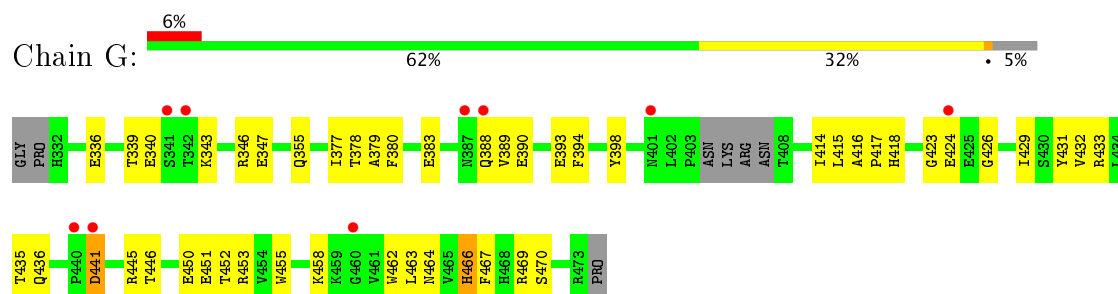
- Molecule 1: CaMKII-B hub



- Molecule 1: CaMKII-B hub



- Molecule 1: CaMKII-B hub



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.97Å 113.97Å 241.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.35 – 3.00 49.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.35-3.00) 92.3 (49.35-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.01Å)	Xtriage
Refinement program	PHENIX (dev_2229: ???)	Depositor
R, $R_{free}$	0.232 , 0.270 0.228 , 0.264	Depositor DCC
$R_{free}$ test set	1662 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 70.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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](#)

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	0.27	0/1122	0.48	0/1521
1	B	0.27	0/1133	0.48	0/1535
1	C	0.25	0/1126	0.47	0/1525
1	D	0.25	0/1114	0.46	0/1508
1	E	0.27	0/1142	0.47	0/1548
1	F	0.26	0/1189	0.47	0/1611
1	G	0.25	0/2266	0.44	0/3070
All	All	0.26	0/9092	0.47	0/12318

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	338	ASP	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	1100	0	1083	16	0
1	B	1111	0	1096	24	0
1	C	1104	0	1089	12	0
1	D	1094	0	1082	12	0
1	E	1118	0	1104	14	0
1	F	1164	0	1149	17	0
1	G	2222	0	2192	37	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
All	All	8925	0	8795	124	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 7.

The worst 5 of 124 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:343:LYS:HB3	1:A:347:GLU:HG3	1.66	0.78
1:F:341:SER:HB3	1:C:341:SER:HB2	1.66	0.77
1:E:441:ASP:OD1	1:E:442:GLY:N	2.19	0.75
1:G:426[B]:GLY:HA3	1:G:455[B]:TRP:O	1.87	0.75
1:G:453[B]:ARG:NH1	1:G:464[B]:ASN:OD1	2.21	0.74

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	133/145 (92%)	129 (97%)	2 (2%)	2 (2%)	12	48
1	B	134/145 (92%)	128 (96%)	5 (4%)	1 (1%)	25	67
1	C	133/145 (92%)	128 (96%)	4 (3%)	1 (1%)	22	64
1	D	132/145 (91%)	126 (96%)	5 (4%)	1 (1%)	22	64
1	E	135/145 (93%)	128 (95%)	6 (4%)	1 (1%)	25	67
1	F	142/145 (98%)	136 (96%)	3 (2%)	3 (2%)	8	38
1	G	268/145 (185%)	244 (91%)	22 (8%)	2 (1%)	25	67
All	All	1077/1015 (106%)	1019 (95%)	47 (4%)	11 (1%)	17	59

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	339	THR
1	F	405	LYS
1	B	402	LEU
1	A	402	LEU
1	F	404	ASN

### 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	124/131 (95%)	120 (97%)	4 (3%)	44	79
1	B	125/131 (95%)	117 (94%)	8 (6%)	20	57
1	C	124/131 (95%)	122 (98%)	2 (2%)	68	90
1	D	123/131 (94%)	122 (99%)	1 (1%)	85	95
1	E	126/131 (96%)	125 (99%)	1 (1%)	85	95
1	F	131/131 (100%)	129 (98%)	2 (2%)	70	91
1	G	250/131 (191%)	248 (99%)	2 (1%)	85	95
All	All	1003/917 (109%)	983 (98%)	20 (2%)	57	87

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	339	THR
1	B	332	HIS
1	B	410	VAL
1	C	402	LEU
1	D	380	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	404	ASN
1	B	448	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	137/145 (94%)	-0.26	2 (1%) 74 47	57, 84, 167, 216	0
1	B	138/145 (95%)	0.09	7 (5%) 29 12	69, 112, 193, 227	0
1	C	137/145 (94%)	0.28	14 (10%) 7 3	58, 116, 171, 206	0
1	D	136/145 (93%)	0.54	18 (13%) 4 1	68, 130, 188, 231	0
1	E	139/145 (95%)	-0.31	2 (1%) 75 49	47, 72, 155, 179	0
1	F	143/145 (98%)	-0.19	7 (4%) 30 12	48, 73, 170, 201	0
1	G	138/145 (95%)	0.62	9 (6%) 20 7	57, 87, 151, 168	0
All	All	968/1015 (95%)	0.10	59 (6%) 22 8	47, 96, 172, 231	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	426	GLY	5.8
1	C	422	LEU	5.3
1	C	427	ALA	4.6
1	G	342[A]	THR	4.6
1	D	460	GLY	4.5

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.