



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 04:11 AM EDT

PDB ID : 6NIT  
Title : Human Argonaute2-miR-122 bound to a target RNA with four central mismatches (bu4)  
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Deposited on : 2018-12-31  
Resolution : 3.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

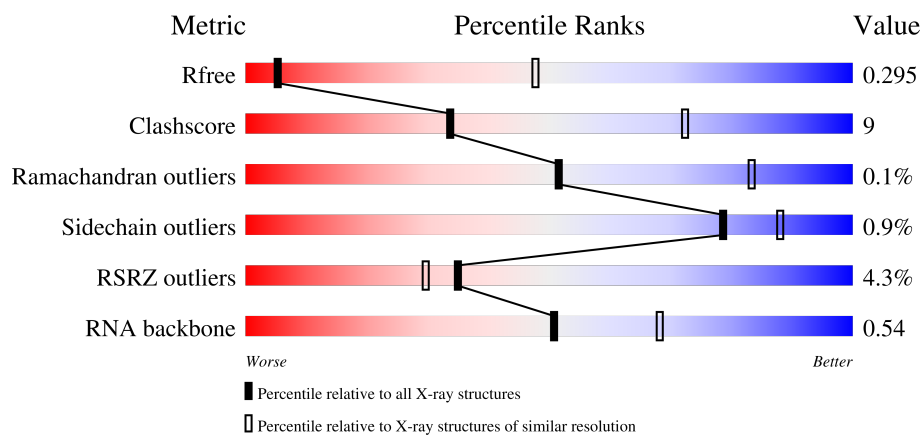
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	859	
1	B	859	
2	C	21	
2	D	21	

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Mol	Chain	Length	Quality of chain
3	E	23	<div><div></div><div>22%</div><div></div><div>70%</div><div></div><div>17%</div><div></div><div>•</div><div>9%</div></div>
3	F	23	<div><div></div><div>30%</div><div></div><div>52%</div><div></div><div>17%</div><div></div><div>13%</div><div></div><div>•</div><div>13%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14206 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 Protein argonaute-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	798	Total	C	N	O	S	0	0	0
			6398	4073	1151	1133	41			
1	B	793	Total	C	N	O	S	0	0	0
			6360	4051	1143	1126	40			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8
A	669	ALA	ASP	engineered mutation	UNP Q9UKV8
A	824	ALA	SER	engineered mutation	UNP Q9UKV8
A	828	ASP	SER	engineered mutation	UNP Q9UKV8
A	831	ASP	SER	engineered mutation	UNP Q9UKV8
A	834	ALA	SER	engineered mutation	UNP Q9UKV8
B	387	ASP	SER	engineered mutation	UNP Q9UKV8
B	669	ALA	ASP	engineered mutation	UNP Q9UKV8
B	824	ALA	SER	engineered mutation	UNP Q9UKV8
B	828	ASP	SER	engineered mutation	UNP Q9UKV8
B	831	ASP	SER	engineered mutation	UNP Q9UKV8
B	834	ALA	SER	engineered mutation	UNP Q9UKV8

- Molecule 2 is a RNA chain called RNA (5'-R(P\*UP\*GP\*GP\*AP\*GP\*UP\*GP\*UP\*GP\*AP\*CP\*AP\*AP\*UP\*GP\*GP\*UP\*GP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			372	163	64	127	18			
2	D	13	Total	C	N	O	P	0	0	0
			267	116	48	90	13			

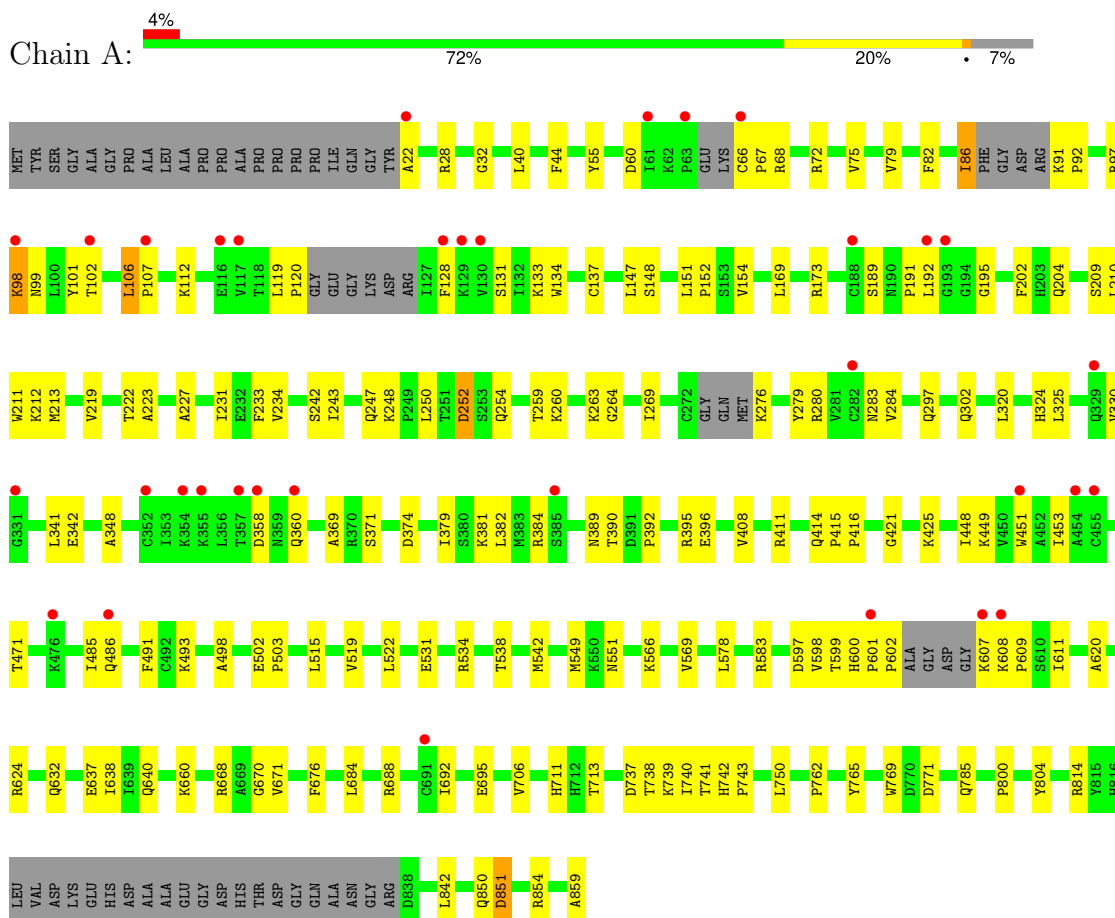
- Molecule 3 is a RNA chain called RNA (5'-R(P\*AP\*AP\*CP\*AP\*CP\*CP\*AP\*UP\*CP\*CP\*AP\*AP\*CP\*AP\*CP\*UP\*CP\*CP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	21	Total 406	C 180	N 73	O 132	P 21	0	0	0
3	F	20	Total 403	C 180	N 74	O 129	P 20	0	0	0

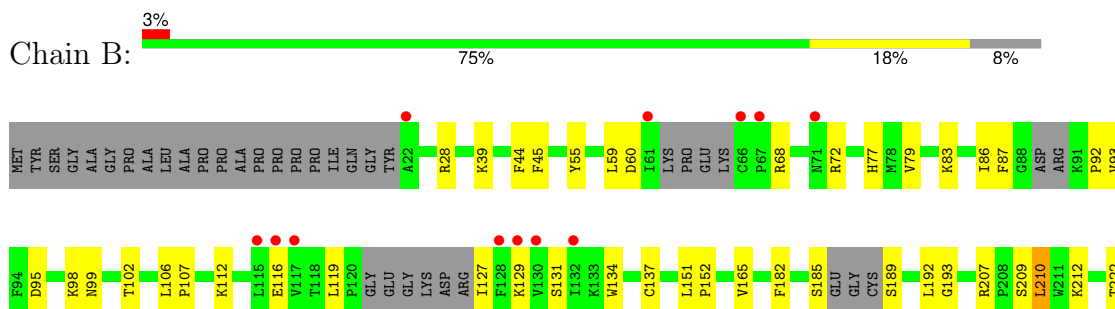
### 3 Residue-property plots

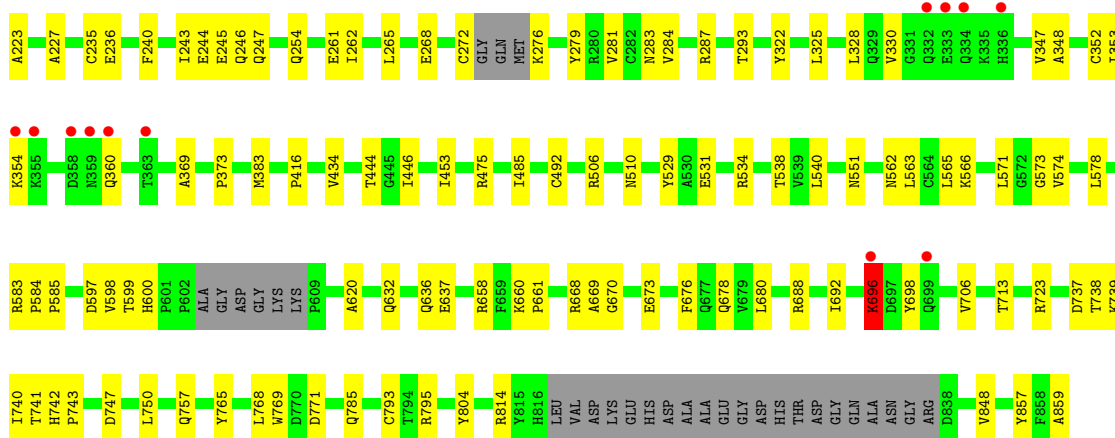
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein argonaute-2



#### • Molecule 1: Protein argonaute-2





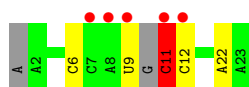
● Molecule 2: RNA (5'-R(P\*UP\*GP\*GP\*AP\*GP\*UP\*GP\*UP\*GP\*AP\*CP\*AP\*AP\*UP\*GP\*G P\*UP\*GP\*UP\*UP\*U)-3')



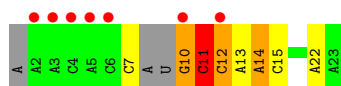
● Molecule 2: RNA (5'-R(P\*UP\*GP\*GP\*AP\*GP\*UP\*GP\*UP\*GP\*AP\*CP\*AP\*AP\*UP\*GP\*G P\*UP\*GP\*UP\*UP\*U)-3')



● Molecule 3: RNA (5'-R(P\*AP\*AP\*CP\*AP\*CP\*CP\*AP\*UP\*CP\*CP\*AP\*AP\*CP\*AP\*CP\*U P\*CP\*CP\*AP\*AP\*A)-3')



● Molecule 3: RNA (5'-R(P\*AP\*AP\*CP\*AP\*CP\*CP\*AP\*UP\*CP\*CP\*AP\*AP\*CP\*AP\*CP\*U P\*CP\*CP\*AP\*AP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.71Å 137.09Å 154.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.30 – 3.80 39.30 – 3.77	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.30-3.80) 98.9 (39.30-3.77)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.243 , 0.294 0.253 , 0.295	Depositor DCC
$R_{free}$ test set	1163 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.9	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6859e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.23	0/6548	0.46	0/8862
1	B	0.24	0/6509	0.45	1/8809 (0.0%)
2	C	0.55	1/414 (0.2%)	0.74	0/641
2	D	0.66	1/297 (0.3%)	0.93	1/459 (0.2%)
3	E	0.23	0/449	0.88	2/689 (0.3%)
3	F	0.19	0/447	0.73	1/688 (0.1%)
All	All	0.26	2/14664 (0.0%)	0.51	5/20148 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-10.54	1.48	1.61
2	D	1	U	OP3-P	-10.29	1.48	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	14	U	P-O3'-C3'	6.68	127.72	119.70
3	E	11	C	P-O3'-C3'	6.36	127.33	119.70
3	E	11	C	OP2-P-O3'	6.12	118.66	105.20
1	B	245	GLU	N-CA-C	-5.88	95.11	111.00
3	F	11	C	P-O3'-C3'	5.35	126.12	119.70

There are no chirality outliers.

There are no planarity outliers.

### 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	6398	0	6461	114	0
1	B	6360	0	6413	106	0
2	C	372	0	181	7	0
2	D	267	0	129	16	0
3	E	406	0	209	4	0
3	F	403	0	210	12	0
All	All	14206	0	13603	236	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 236 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:566:LYS:NZ	1:B:859:ALA:OXT	1.77	1.18
1:B:551:ASN:ND2	2:D:2:G:OP2	2.02	0.91
1:B:531:GLU:OE2	1:B:534:ARG:NH1	2.06	0.88
1:A:384:ARG:NH1	1:B:658:ARG:HD3	1.91	0.84
1:A:551:ASN:ND2	2:C:2:G:OP2	2.11	0.83

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	784/859 (91%)	747 (95%)	36 (5%)	1 (0%)	51	83
1	B	777/859 (90%)	738 (95%)	38 (5%)	1 (0%)	51	83
All	All	1561/1718 (91%)	1485 (95%)	74 (5%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	696	LYS
1	A	98	LYS

### 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	708/749 (94%)	701 (99%)	7 (1%)	76	86
1	B	703/749 (94%)	698 (99%)	5 (1%)	84	91
All	All	1411/1498 (94%)	1399 (99%)	12 (1%)	78	88

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	HIS
1	B	137	CYS
1	B	804	TYR
1	B	210	LEU
1	A	252	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	729	ASN
1	B	324	HIS
1	A	254	GLN
1	A	204	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	15/21 (71%)	6 (40%)	2 (13%)
2	D	11/21 (52%)	3 (27%)	2 (18%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	16/23 (69%)	1 (6%)	1 (6%)
3	F	17/23 (73%)	3 (17%)	2 (11%)
All	All	59/88 (67%)	13 (22%)	7 (11%)

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	13	A
2	C	14	U
2	C	15	G
2	C	17	U
2	C	18	G

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	14	U
3	E	11	C
3	F	11	C
3	F	10	G
2	D	13	A

## 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 monosaccharides 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	798/859 (92%)	0.19	34 (4%) 35 30	61, 111, 190, 247	0
1	B	793/859 (92%)	0.05	24 (3%) 50 40	53, 97, 175, 249	0
2	C	18/21 (85%)	0.93	1 (5%) 24 20	82, 142, 270, 275	0
2	D	13/21 (61%)	0.64	1 (7%) 13 11	76, 90, 188, 203	0
3	E	21/23 (91%)	0.93	5 (23%) 0 0	115, 184, 224, 245	0
3	F	20/23 (86%)	1.38	7 (35%) 0 0	83, 157, 271, 299	0
All	All	1663/1806 (92%)	0.16	72 (4%) 35 30	53, 104, 190, 299	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	CYS	5.6
1	B	129	LYS	5.1
1	B	334	GLN	4.8
1	A	66	CYS	4.7
1	B	116	GLU	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 monosaccharides 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.