



# Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2019 – 04:10 AM EDT

PDB ID : 6N4O  
Title : Human Argonaute2-miR-122 bound to a seed and supplementary paired target  
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Deposited on : 2018-11-19  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

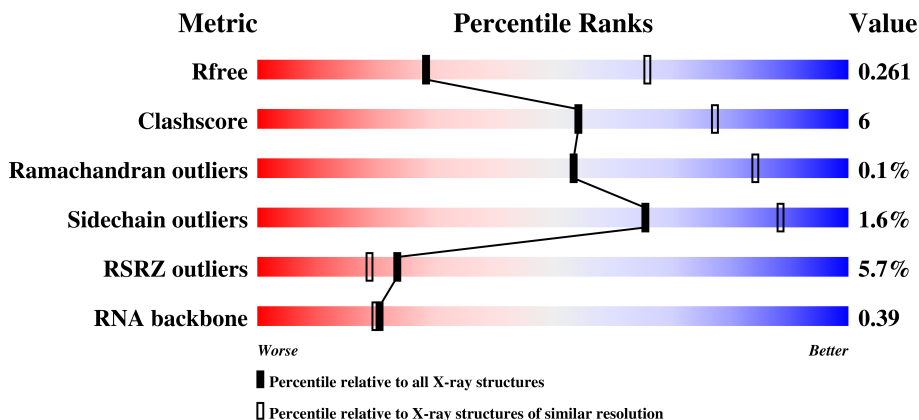
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)
RNA backbone	2636	1059 (3.20-2.60)

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	859	<div> <div>5%</div> <div>79%</div> <div>13%</div> <div>7%</div> </div>
2	C	21	<div> <div>10%</div> <div>24%</div> <div>52%</div> <div>14%</div> <div>10%</div> </div>
3	D	18	<div> <div>11%</div> <div>61%</div> <div>17%</div> <div>22%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7064 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	796	Total	C	N	O	S	0	0	0
			6384	4066	1151	1127	40			

There are 6 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

- 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	19	Total	C	N	O	P	0	0	0
			411	182	72	138	19			

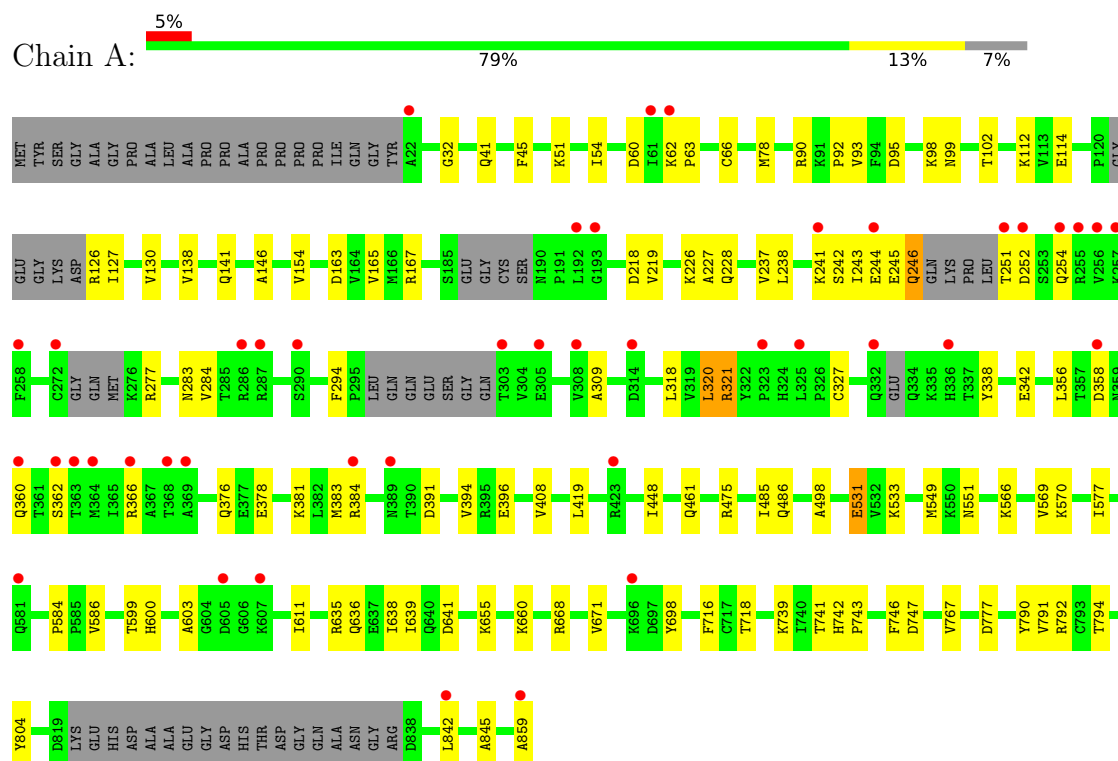
- Molecule 3 is a RNA chain called RNA (5'-R(\*CP\*CP\*AP\*UP\*UP\*GP\*UP\*CP\*AP\*CP\*AP\*CP\*UP\*CP\*CP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			269	121	44	91	13			

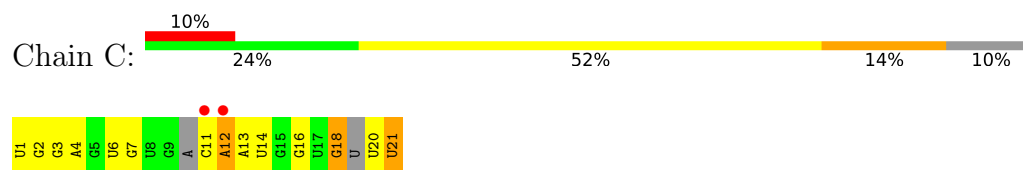
### 3 Residue-property plots [i](#)

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: 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 3: RNA (5'-R(\*CP\*CP\*AP\*UP\*UP\*GP\*UP\*CP\*AP\*CP\*AP\*CP\*UP\*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, $\alpha$ , $\beta$ , $\gamma$	66.13Å 66.33Å 247.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 2.90 39.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.00-2.90) 96.4 (39.65-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.207 , 0.257 0.210 , 0.261	Depositor DCC
$R_{free}$ test set	1236 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.23	0/6533	0.41	0/8839
2	C	0.56	1/457 (0.2%)	0.74	0/705
3	D	0.21	0/297	0.76	0/457
All	All	0.26	1/7287 (0.0%)	0.46	0/10001

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-10.81	1.48	1.61

There are no bond angle outliers.

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	6384	0	6447	69	0
2	C	411	0	205	13	0
3	D	269	0	142	2	0
All	All	7064	0	6794	78	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 6.

All (78) 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:163:ASP:OD2	1:A:167:ARG:NH1	1.98	0.96
1:A:112:LYS:NZ	1:A:114:GLU:OE2	2.13	0.82
2:C:6:U:HO2'	2:C:7:G:H8	1.35	0.72
1:A:90:ARG:NH1	1:A:396:GLU:OE2	2.24	0.70
1:A:60:ASP:OD1	1:A:98:LYS:NZ	2.26	0.67
1:A:566:LYS:NZ	1:A:859:ALA:HB1	2.09	0.66
1:A:570:LYS:HE3	1:A:859:ALA:HA	1.76	0.65
1:A:126:ARG:HD2	2:C:18:G:H1	1.61	0.65
1:A:636:GLN:HG2	1:A:638:ILE:HG22	1.79	0.64
1:A:356:LEU:HB3	1:A:360:GLN:HG2	1.80	0.63
2:C:20:U:O2'	2:C:21:U:O5'	2.18	0.61
1:A:603:ALA:HB2	1:A:635:ARG:NH1	2.17	0.60
2:C:20:U:O2'	2:C:21:U:O4'	2.18	0.59
1:A:461:GLN:HB2	1:A:549:MET:HE1	1.87	0.56
1:A:448:ILE:HD13	1:A:485:ILE:HG12	1.87	0.55
1:A:842:LEU:HD22	1:A:845:ALA:HB2	1.89	0.55
1:A:54:ILE:HB	1:A:138:VAL:HB	1.89	0.55
1:A:318:LEU:HG	1:A:320:LEU:H	1.72	0.55
1:A:237:VAL:HG12	1:A:238:LEU:HD22	1.88	0.55
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.90	0.54
1:A:45:PHE:CZ	1:A:383:MET:HG3	2.42	0.54
1:A:41:GLN:HG3	1:A:718:THR:HG22	1.90	0.53
1:A:93:VAL:HG11	1:A:165:VAL:HA	1.89	0.53
1:A:475:ARG:NH1	1:A:486:GLN:O	2.41	0.53
1:A:146:ALA:HB1	1:A:154:VAL:HG22	1.91	0.52
1:A:62:LYS:HB3	1:A:63:PRO:HD3	1.91	0.51
1:A:741:THR:OG1	1:A:742:HIS:N	2.44	0.51
1:A:551:ASN:ND2	2:C:2:G:OP2	2.39	0.51
1:A:242:SER:HB2	1:A:244:GLU:OE2	2.12	0.50
1:A:566:LYS:HZ2	1:A:859:ALA:HB1	1.76	0.50
1:A:660:LYS:NZ	1:A:660:LYS:HB3	2.27	0.50
1:A:358:ASP:OD1	3:D:11:A:H5''	2.11	0.49
1:A:419:LEU:HD23	1:A:577:ILE:HD11	1.94	0.49
1:A:126:ARG:HG2	1:A:127:ILE:H	1.76	0.49
1:A:251:THR:OG1	1:A:252:ASP:N	2.46	0.49
1:A:639:ILE:HG13	1:A:668:ARG:HH21	1.77	0.49
1:A:584:PRO:HB2	1:A:586:VAL:HG23	1.95	0.49
1:A:741:THR:OG1	1:A:747:ASP:OD1	2.30	0.49
1:A:241:LYS:HB2	1:A:245:GLU:OE2	2.12	0.49
1:A:277:ARG:NH1	2:C:18:G:C8	2.81	0.48
1:A:277:ARG:NH1	2:C:18:G:H8	2.11	0.48
1:A:498:ALA:HB1	1:A:531:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:HB2	1:A:99:ASN:HB2	1.95	0.47
1:A:226:LYS:HG2	1:A:228:GLN:HG3	1.96	0.47
1:A:381:LYS:HD3	1:A:384:ARG:HD3	1.96	0.47
2:C:6:U:O2'	2:C:7:G:H8	1.97	0.47
2:C:12:A:H2'	2:C:13:A:C8	2.49	0.47
3:D:2:C:H2'	3:D:3:A:C8	2.50	0.46
2:C:3:G:H2'	2:C:4:A:C8	2.50	0.46
1:A:600:HIS:HB3	1:A:635:ARG:HD2	1.98	0.46
1:A:309:ALA:HA	1:A:320:LEU:HD13	1.99	0.45
1:A:391:ASP:OD2	1:A:394:VAL:HG23	2.16	0.45
1:A:283:ASN:OD1	1:A:284:VAL:N	2.47	0.45
1:A:32:GLY:HA2	1:A:777:ASP:OD2	2.17	0.45
1:A:378:GLU:HA	1:A:381:LYS:HB2	1.99	0.44
2:C:11:C:O3'	2:C:12:A:H4'	2.18	0.44
1:A:51:LYS:HB3	1:A:141:GLN:HG2	2.01	0.43
1:A:746:PHE:HB3	1:A:767:VAL:HB	2.00	0.43
1:A:376:GLN:HB2	1:A:716:PHE:CD1	2.53	0.43
1:A:408:VAL:HG23	1:A:739:LYS:HB2	2.00	0.43
1:A:842:LEU:HA	1:A:842:LEU:HD23	1.85	0.43
2:C:13:A:H2'	2:C:14:U:C6	2.55	0.42
1:A:655:LYS:HB3	1:A:655:LYS:HE2	1.85	0.42
1:A:318:LEU:HG	1:A:320:LEU:N	2.35	0.42
1:A:327:CYS:SG	1:A:338:TYR:HB3	2.60	0.42
1:A:294:PHE:CE1	2:C:21:U:H2'	2.55	0.42
1:A:362:SER:HB3	1:A:366:ARG:HH12	1.85	0.41
1:A:569:VAL:HG21	1:A:791:VAL:HB	2.02	0.41
1:A:533:LYS:HD3	1:A:533:LYS:HA	1.88	0.41
1:A:660:LYS:NZ	1:A:698:TYR:CD1	2.89	0.41
1:A:790:TYR:CE2	1:A:792:ARG:HB2	2.56	0.41
1:A:245:GLU:O	1:A:246:GLN:HG2	2.20	0.41
1:A:742:HIS:CG	1:A:743:PRO:HD2	2.55	0.41
1:A:218:ASP:OD1	1:A:219:VAL:N	2.52	0.41
1:A:611:ILE:HG13	1:A:611:ILE:H	1.78	0.40
1:A:668:ARG:NH1	1:A:671:VAL:HG23	2.37	0.40
1:A:321:ARG:HD2	1:A:342:GLU:OE2	2.22	0.40
1:A:78:MET:SD	1:A:130:VAL:HG21	2.61	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	780/859 (91%)	732 (94%)	47 (6%)	1 (0%)	53	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ALA

### 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	704/749 (94%)	693 (98%)	11 (2%)	65	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	CYS
1	A	243	ILE
1	A	246	GLN
1	A	254	GLN
1	A	320	LEU
1	A	321	ARG
1	A	531	GLU
1	A	599	THR
1	A	641	ASP
1	A	794	THR

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Mol	Chain	Res	Type
1	A	804	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	16/21 (76%)	4 (25%)	0
3	D	11/18 (61%)	0	0
All	All	27/39 (69%)	4 (14%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	12	A
2	C	16	G
2	C	18	G
2	C	21	U

There are no RNA pucker outliers to report.

## 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

### 6.1 Protein, DNA and RNA chains

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	796/859 (92%)	0.12	43 (5%) 26 21	26, 56, 135, 187	0
2	C	19/21 (90%)	0.82	2 (10%) 6 4	34, 118, 181, 205	0
3	D	14/18 (77%)	0.82	2 (14%) 2 2	60, 98, 165, 170	0
All	All	829/898 (92%)	0.15	47 (5%) 24 19	26, 57, 141, 205	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	GLN	6.7
1	A	360	GLN	5.6
1	A	257	LYS	5.4
1	A	323	PRO	4.5
1	A	303	THR	4.2
1	A	286	ARG	4.0
1	A	62	LYS	3.4
1	A	251	THR	3.2
1	A	358	ASP	3.2
1	A	314	ASP	3.2
1	A	364	MET	3.2
1	A	368	THR	3.1
3	D	1	C	3.1
1	A	607	LYS	3.0
1	A	244	GLU	3.0
1	A	252	ASP	3.0
2	C	11	C	2.9
2	C	12	A	2.9
1	A	193	GLY	2.9
3	D	6	G	2.8
1	A	287	ARG	2.8
1	A	336	HIS	2.6
1	A	369	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	389	ASN	2.5
1	A	241	LYS	2.5
1	A	423	ARG	2.5
1	A	325	LEU	2.5
1	A	254	GLN	2.4
1	A	366	ARG	2.4
1	A	308	VAL	2.4
1	A	22	ALA	2.4
1	A	605	ASP	2.3
1	A	61	ILE	2.3
1	A	192	LEU	2.3
1	A	256	VAL	2.3
1	A	384	ARG	2.3
1	A	363	THR	2.2
1	A	290	SER	2.2
1	A	305	GLU	2.2
1	A	842	LEU	2.2
1	A	272	CYS	2.2
1	A	696	LYS	2.1
1	A	255	ARG	2.1
1	A	581	GLN	2.1
1	A	362	SER	2.1
1	A	859	ALA	2.0
1	A	258	PHE	2.0

## 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.