



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:13 pm BST

PDB ID : 4PER  
Title : Structure of Gallus gallus ribonuclease inhibitor complexed with Gallus gallus ribonuclease I  
Authors : Bianchetti, C.M.; Lomax, J.E.; Raines, R.T.; Fox, B.G.  
Deposited on : 2014-04-24  
Resolution : 1.92 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	:	2.11
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)	:	2.11

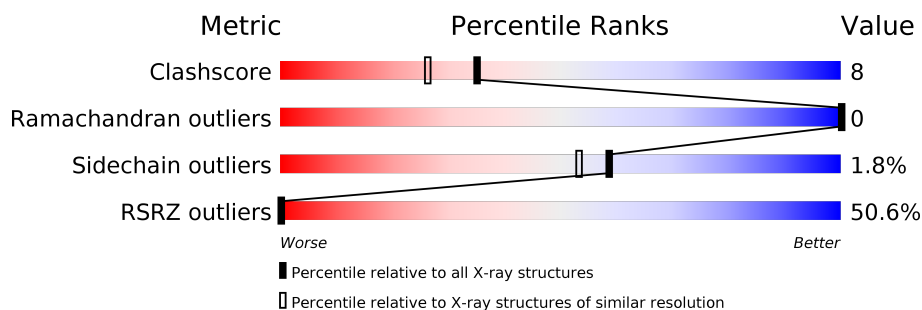
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 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	460	
2	B	113	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4636 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 Ribonuclease Inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	458	3533	2198	596	701	38	0	10	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP Q5ZIIY8
A	-2	PHE	-	expression tag	UNP Q5ZIIY8
A	-1	GLN	-	expression tag	UNP Q5ZIIY8
A	0	GLY	-	expression tag	UNP Q5ZIIY8
A	10	ILE	MET	conflict	UNP Q5ZIIY8

- Molecule 2 is a protein called Angiogenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	109	870	538	171	154	7	0	0	0

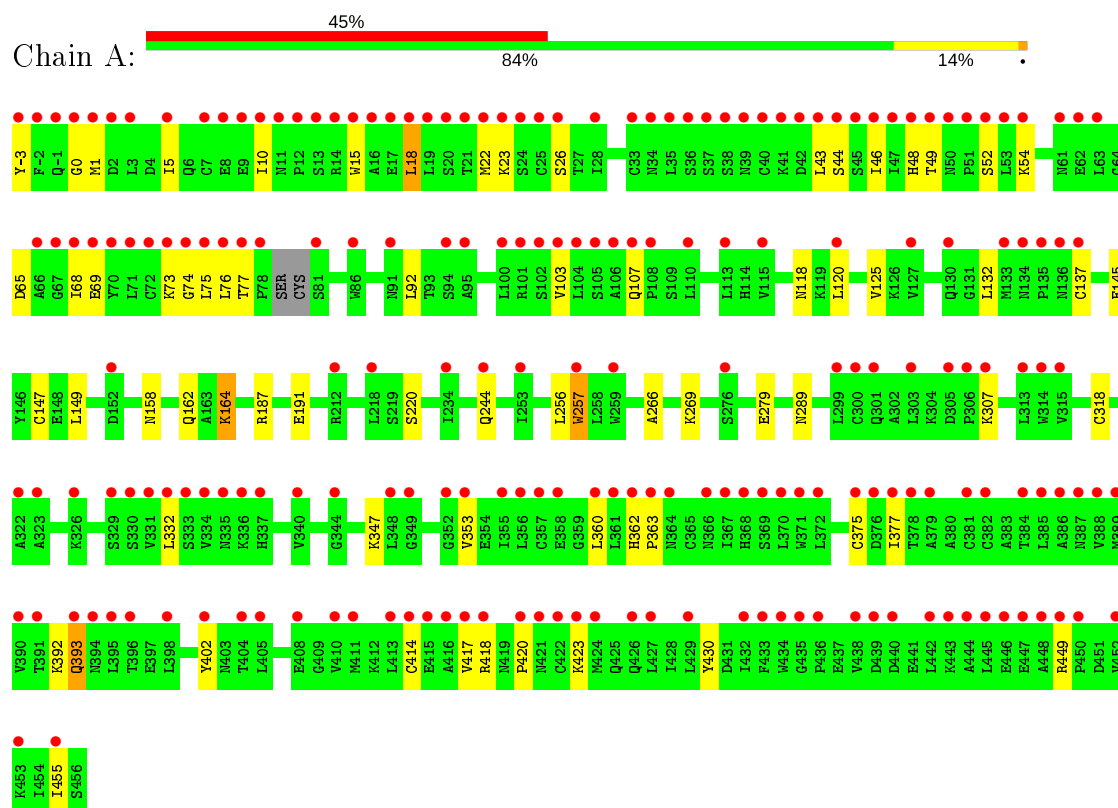
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total	O	0	0
			195	195		
3	B	38	Total	O	0	0
			38	38		

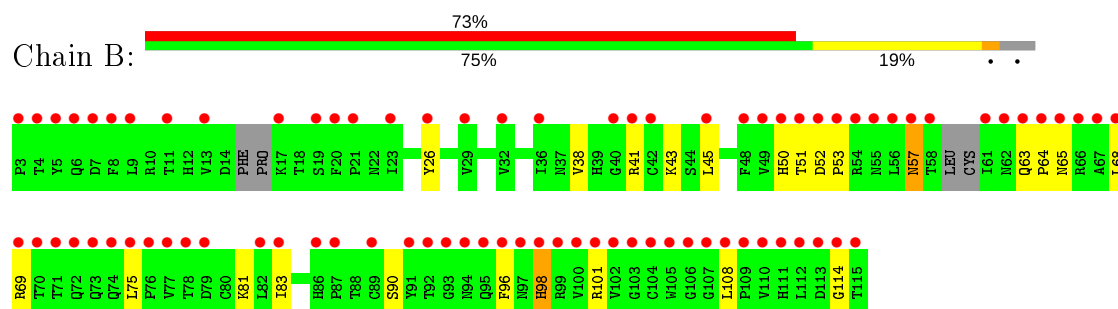
### 3 Residue-property plots [i](#)

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: Ribonuclease Inhibitor



#### • Molecule 2: Angiogenin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.66Å 84.54Å 121.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 1.92 41.96 – 1.77	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.81-1.92) 91.3 (41.96-1.77)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.202 , 0.254 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	1.6	Xtriage
Anisotropy	2.584	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 60.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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	0.45	0/3607	0.58	2/4886 (0.0%)
2	B	0.39	0/889	0.61	0/1205
All	All	0.44	0/4496	0.59	2/6091 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	TRP	CA-CB-CG	-5.68	102.91	113.70
1	A	393	GLN	CA-CB-CG	5.42	125.31	113.40

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	3533	0	3583	57	0
2	B	870	0	851	24	0
3	A	195	0	0	3	0
3	B	38	0	0	0	0
All	All	4636	0	4434	72	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 8.

All (72) 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)
2:B:53:PRO:O	2:B:57:ASN:ND2	2.06	0.87
2:B:57:ASN:H	2:B:57:ASN:HD22	1.27	0.82
1:A:455:ILE:HD12	2:B:41:ARG:HH11	1.46	0.79
1:A:75:LEU:HD12	1:A:103:VAL:HG22	1.67	0.77
2:B:57:ASN:N	2:B:57:ASN:HD22	1.82	0.76
2:B:38:VAL:HG23	2:B:41:ARG:HH21	1.53	0.74
1:A:23:LYS:NZ	1:A:49:THR:OG1	2.26	0.68
1:A:257:TRP:CZ3	2:B:83:ILE:O	2.49	0.66
1:A:5:ILE:HD11	1:A:18:LEU:HD21	1.79	0.65
1:A:75:LEU:HD11	1:A:103:VAL:HG13	1.78	0.65
1:A:402:TYR:OH	2:B:45:LEU:O	2.15	0.64
2:B:101:ARG:HB3	2:B:114:GLY:HA3	1.81	0.62
1:A:10:ILE:HG21	1:A:15:TRP:HE3	1.64	0.62
2:B:96:PHE:HB3	2:B:98:HIS:ND1	2.15	0.61
1:A:48:HIS:CD2	1:A:77:THR:HG22	2.35	0.61
1:A:402:TYR:OH	2:B:43:LYS:HE2	2.02	0.58
1:A:75:LEU:HD13	1:A:75:LEU:O	2.03	0.58
1:A:257:TRP:HZ3	2:B:83:ILE:O	1.89	0.55
1:A:256:LEU:C	1:A:257:TRP:HD1	2.10	0.54
1:A:65:ASP:O	1:A:69:GLU:HG3	2.07	0.54
1:A:455:ILE:HD12	2:B:41:ARG:NH1	2.20	0.54
1:A:393:GLN:HE22	1:A:423:LYS:HE2	1.73	0.53
1:A:393:GLN:NE2	1:A:423:LYS:HG2	2.24	0.53
1:A:455:ILE:HG23	2:B:41:ARG:HH11	1.74	0.52
1:A:43:LEU:HA	1:A:46:ILE:HD12	1.92	0.52
1:A:75:LEU:O	1:A:107:GLN:NE2	2.44	0.51
1:A:393:GLN:NE2	1:A:423:LYS:HE2	2.27	0.50
1:A:158:ASN:O	1:A:162:GLN:HG2	2.11	0.50
1:A:417:VAL:O	1:A:449:ARG:HD3	2.12	0.50
1:A:75:LEU:CD1	1:A:103:VAL:HG13	2.41	0.50
1:A:18:LEU:O	1:A:22:MET:HG3	2.11	0.49
1:A:0:GLY:HA3	1:A:26:SER:HB2	1.94	0.49
1:A:244:GLN:OE1	3:A:593:HOH:O	2.20	0.48
2:B:63:GLN:HG2	2:B:69:ARG:HD2	1.95	0.48
2:B:26:TYR:OH	2:B:50:HIS:HE1	1.97	0.48
1:A:347:LYS:HE2	1:A:347:LYS:HB3	1.56	0.47
1:A:332:LEU:HD13	1:A:360:LEU:HD23	1.96	0.47
2:B:83:ILE:HG12	2:B:90:SER:O	2.14	0.47
1:A:257:TRP:CD1	1:A:257:TRP:N	2.80	0.47
1:A:187:ARG:NH1	1:A:191:GLU:OE2	2.47	0.47
1:A:73:LYS:O	1:A:76:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:VAL:HG21	1:A:377:ILE:HG21	1.97	0.46
1:A:10:ILE:HG21	1:A:15:TRP:CE3	2.47	0.46
2:B:57:ASN:ND2	2:B:57:ASN:N	2.57	0.46
1:A:125:VAL:HG21	1:A:149:LEU:HD21	1.98	0.46
1:A:187:ARG:NH2	3:A:501:HOH:O	2.21	0.46
1:A:455:ILE:HG23	2:B:41:ARG:NH1	2.31	0.45
2:B:51:THR:HG21	2:B:75:LEU:HD13	1.98	0.45
1:A:266:ALA:O	1:A:269:LYS:HG3	2.17	0.45
1:A:256:LEU:C	1:A:257:TRP:CD1	2.90	0.44
1:A:137:CYS:SG	1:A:164:LYS:HE3	2.57	0.44
1:A:44:SER:O	1:A:74:GLY:HA3	2.17	0.43
1:A:132:LEU:O	1:A:164:LYS:HE2	2.18	0.43
1:A:414:CYS:O	1:A:418:ARG:HG3	2.18	0.43
1:A:392:LYS:HA	1:A:392:LYS:HD2	1.78	0.43
1:A:420:PRO:O	1:A:423:LYS:NZ	2.50	0.43
1:A:68:ILE:HD13	1:A:92:LEU:HD21	2.01	0.43
2:B:45:LEU:HD22	2:B:81:LYS:HE2	2.00	0.43
1:A:120:LEU:HD23	1:A:147:CYS:SG	2.59	0.42
1:A:-3:TYR:N	3:A:507:HOH:O	2.52	0.42
1:A:362:HIS:O	1:A:392:LYS:NZ	2.52	0.42
2:B:63:GLN:HB3	2:B:64:PRO:HD2	2.01	0.42
2:B:108:LEU:HA	2:B:108:LEU:HD23	1.71	0.41
1:A:362:HIS:HA	1:A:363:PRO:HD3	1.90	0.41
1:A:289:ASN:O	1:A:318:CYS:HA	2.20	0.41
1:A:430:TYR:CG	2:B:43:LYS:HE3	2.55	0.41
1:A:375[B]:CYS:SG	1:A:377:ILE:HG23	2.60	0.41
1:A:52:SER:O	1:A:54:LYS:HG3	2.21	0.41
1:A:118:ASN:O	1:A:120:LEU:HD22	2.21	0.41
2:B:68:LEU:HD13	2:B:101:ARG:HH21	1.86	0.41
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.66	0.40
1:A:279:GLU:HG3	1:A:307:LYS:HG2	2.02	0.40

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	464/460 (101%)	452 (97%)	12 (3%)	0	100	100
2	B	103/113 (91%)	97 (94%)	6 (6%)	0	100	100
All	All	567/573 (99%)	549 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	415/407 (102%)	409 (99%)	6 (1%)	67	63
2	B	99/103 (96%)	95 (96%)	4 (4%)	31	21
All	All	514/510 (101%)	504 (98%)	10 (2%)	59	51

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	LEU
1	A	145	GLU
1	A	164	LYS
1	A	220[A]	SER
1	A	220[B]	SER
2	B	52	ASP
2	B	57	ASN
2	B	65	ASN
2	B	98	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	393	GLN
2	B	57	ASN

### 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 [i](#)

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	458/460 (99%)	2.32	205 (44%) <b>0</b> <b>0</b>	5, 27, 50, 64	0
2	B	109/113 (96%)	3.63	82 (75%) <b>0</b> <b>0</b>	20, 36, 69, 76	0
All	All	567/573 (98%)	2.57	287 (50%) <b>0</b> <b>0</b>	5, 29, 58, 76	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	ILE	12.7
2	B	67	ALA	11.9
2	B	58	THR	11.7
1	A	18	LEU	11.1
1	A	78	PRO	9.8
1	A	77	THR	9.5
1	A	-1	GLN	9.1
1	A	76	LEU	8.8
1	A	-3	TYR	8.6
2	B	54	ARG	8.5
2	B	68	LEU	8.4
1	A	15	TRP	8.2
1	A	10	ILE	8.2
1	A	13	SER	8.0
2	B	4	THR	7.7
2	B	108	LEU	7.7
1	A	402	TYR	7.5
2	B	65	ASN	7.5
2	B	55	ASN	7.4
2	B	62	ASN	7.3
1	A	11	ASN	7.2
1	A	19	LEU	6.9
2	B	114	GLY	6.8
2	B	69	ARG	6.7

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Mol	Chain	Res	Type	RSRZ
2	B	102	VAL	6.4
2	B	106	GLY	6.3
1	A	-2	PHE	6.2
1	A	41	LYS	6.2
1	A	433	PHE	6.2
2	B	99	ARG	6.2
1	A	75	LEU	6.0
1	A	106	ALA	5.9
1	A	404	THR	5.8
1	A	47	ILE	5.8
1	A	390	VAL	5.7
2	B	64	PRO	5.7
2	B	63	GLN	5.6
2	B	77	VAL	5.6
2	B	115	THR	5.6
1	A	394	ASN	5.6
1	A	40	CYS	5.5
1	A	38	SER	5.4
1	A	9	GLU	5.3
1	A	43	LEU	5.3
1	A	20	SER	5.3
2	B	52	ASP	5.3
1	A	418	ARG	5.3
2	B	98	HIS	5.3
1	A	33	CYS	5.2
1	A	16	ALA	5.2
2	B	105	TRP	5.2
2	B	50	HIS	5.2
1	A	448	ALA	5.1
1	A	36	SER	5.1
1	A	257	TRP	5.0
2	B	72	GLN	5.0
1	A	48	HIS	5.0
2	B	57	ASN	5.0
2	B	107	GLY	5.0
1	A	2	ASP	4.9
1	A	21	THR	4.9
2	B	3	PRO	4.9
2	B	76	PRO	4.9
1	A	70	TYR	4.8
1	A	364	ASN	4.7
1	A	73	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	13	VAL	4.6
2	B	56	LEU	4.6
1	A	450	PRO	4.6
1	A	71	LEU	4.5
1	A	417	VAL	4.5
1	A	135	PRO	4.5
1	A	63	LEU	4.4
1	A	445	LEU	4.4
2	B	96	PHE	4.4
1	A	23	LYS	4.4
2	B	112	LEU	4.4
1	A	361	LEU	4.3
1	A	340	VAL	4.3
1	A	363	PRO	4.3
1	A	393	GLN	4.2
1	A	415	GLU	4.2
2	B	71	THR	4.2
1	A	51	PRO	4.2
2	B	104	CYS	4.2
1	A	0	GLY	4.2
1	A	17	GLU	4.2
1	A	449	ARG	4.2
1	A	443	LYS	4.1
1	A	360	LEU	4.1
1	A	67	GLY	4.1
1	A	334	VAL	4.0
2	B	74	GLN	4.0
2	B	97	ASN	4.0
1	A	336	LYS	4.0
1	A	35	LEU	4.0
1	A	388	VAL	4.0
1	A	410	VAL	4.0
2	B	51	THR	4.0
1	A	44	SER	4.0
2	B	53	PRO	3.9
1	A	49	THR	3.9
1	A	452	VAL	3.9
1	A	52	SER	3.8
1	A	1	MET	3.8
1	A	24	SER	3.8
1	A	26	SER	3.8
1	A	420	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	438	VAL	3.8
2	B	9	LEU	3.7
1	A	314	TRP	3.7
1	A	371	TRP	3.7
1	A	103	VAL	3.7
1	A	333	SER	3.7
2	B	7	ASP	3.7
1	A	136	ASN	3.6
1	A	12	PRO	3.6
1	A	68	ILE	3.6
1	A	3	LEU	3.6
2	B	100	VAL	3.6
2	B	78	THR	3.6
2	B	103	GLY	3.6
1	A	446	GLU	3.5
1	A	307	LYS	3.5
1	A	335	ASN	3.5
1	A	442	LEU	3.5
1	A	34[A]	ASN	3.5
1	A	434	TRP	3.5
2	B	19	SER	3.5
1	A	323	ALA	3.5
1	A	444	ALA	3.5
2	B	66	ARG	3.5
1	A	72	CYS	3.4
1	A	22	MET	3.4
1	A	368[A]	HIS	3.4
2	B	86	HIS	3.4
2	B	109	PRO	3.4
1	A	306	PRO	3.4
1	A	37	SER	3.4
1	A	46	ILE	3.4
1	A	432	ILE	3.4
1	A	369	SER	3.3
1	A	53	LEU	3.3
2	B	5	TYR	3.3
1	A	322	ALA	3.3
1	A	391	THR	3.3
2	B	48	PHE	3.3
2	B	73	GLN	3.3
1	A	421	ASN	3.3
1	A	382	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	83	ILE	3.2
1	A	120	LEU	3.2
1	A	331	VAL	3.2
1	A	329	SER	3.2
1	A	385	LEU	3.2
2	B	75	LEU	3.2
1	A	389	MET	3.2
1	A	332	LEU	3.1
1	A	61	ASN	3.1
1	A	423	LYS	3.1
1	A	100	LEU	3.1
1	A	14	ARG	3.1
1	A	424	MET	3.1
1	A	439	ASP	3.1
2	B	45	LEU	3.1
1	A	413	LEU	3.0
2	B	8	PHE	3.0
2	B	36	ILE	3.0
1	A	39	ASN	3.0
1	A	326	LYS	3.0
2	B	29	VAL	3.0
1	A	447	GLU	3.0
1	A	25	CYS	3.0
2	B	49	VAL	3.0
1	A	66	ALA	2.9
1	A	411	MET	2.9
1	A	426	GLN	2.9
1	A	62	GLU	2.9
1	A	69	GLU	2.9
1	A	42	ASP	2.9
2	B	21	PRO	2.8
1	A	8	GLU	2.8
1	A	74	GLY	2.8
1	A	440	ASP	2.8
2	B	113	ASP	2.8
1	A	81	SER	2.8
1	A	102	SER	2.8
1	A	315	VAL	2.8
2	B	20	PHE	2.7
1	A	435	GLY	2.7
2	B	93	GLY	2.7
1	A	104	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLN	2.7
1	A	398	LEU	2.7
2	B	6	GLN	2.7
1	A	386	ALA	2.7
1	A	91[A]	ASN	2.7
1	A	110	LEU	2.7
1	A	5	ILE	2.7
1	A	387	ASN	2.7
2	B	23	ILE	2.7
1	A	54	LYS	2.7
1	A	45	SER	2.7
1	A	101	ARG	2.6
1	A	366	ASN	2.6
1	A	416	ALA	2.6
2	B	95	GLN	2.6
2	B	32	VAL	2.6
1	A	105	SER	2.6
2	B	87	PRO	2.6
1	A	375[A]	CYS	2.6
2	B	70	THR	2.6
1	A	384	THR	2.5
1	A	107	GLN	2.5
1	A	305	ASP	2.5
1	A	7	CYS	2.5
1	A	427	LEU	2.5
2	B	82	LEU	2.5
1	A	301	GLN	2.5
1	A	370	LEU	2.5
1	A	376	ASP	2.5
2	B	17	LYS	2.4
2	B	89	CYS	2.4
2	B	110	VAL	2.4
1	A	436	PRO	2.4
2	B	26	TYR	2.4
1	A	86	TRP	2.4
1	A	414	CYS	2.4
2	B	41	ARG	2.3
1	A	379	ALA	2.3
1	A	127	VAL	2.3
1	A	300	CYS	2.3
1	A	429	LEU	2.3
1	A	94	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	2.3
2	B	101	ARG	2.3
1	A	396	THR	2.3
2	B	92	THR	2.3
1	A	405	LEU	2.3
1	A	353	VAL	2.3
2	B	11	THR	2.2
1	A	378	THR	2.2
2	B	111	HIS	2.2
1	A	115	VAL	2.2
1	A	137	CYS	2.2
2	B	42	CYS	2.2
1	A	134	ASN	2.2
1	A	212	ARG	2.2
1	A	28	ILE	2.2
1	A	372	LEU	2.2
1	A	344	GLY	2.2
1	A	358	GLU	2.2
1	A	381	CYS	2.2
1	A	377	ILE	2.1
1	A	455	ILE	2.1
1	A	330	SER	2.1
1	A	357	CYS	2.1
1	A	362	HIS	2.1
1	A	349	GLY	2.1
1	A	356	LEU	2.1
1	A	276[A]	SER	2.1
1	A	355	ILE	2.1
1	A	50	ASN	2.1
2	B	79	ASP	2.1
2	B	94	ASN	2.1
2	B	91	TYR	2.1
1	A	133	MET	2.1
1	A	253	ILE	2.1
1	A	422	CYS	2.1
1	A	303	LEU	2.1
1	A	348	LEU	2.1
1	A	244	GLN	2.1
1	A	152	ASP	2.1
1	A	113	LEU	2.1
1	A	218	LEU	2.1
1	A	408	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	2.0
1	A	453	LYS	2.0
1	A	299	LEU	2.0
1	A	395	LEU	2.0
1	A	337	HIS	2.0
1	A	95	ALA	2.0
1	A	352	GLY	2.0
2	B	40	GLY	2.0
1	A	259	TRP	2.0
1	A	313	LEU	2.0
1	A	367	ILE	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.