

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 08:02 PM EDT

PDB ID : 1YYW

Title: Crystal structure of RNase III from Aquifex aeolicus complexed with double

stranded RNA at 2.8-Angstrom Resolution

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Deposited on : 2005-02-25

Resolution : 2.80 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

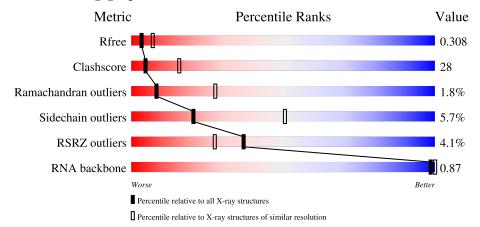
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\bf Similar \ resolution} \\ (\#{\bf Entries, \ resolution \ range(\AA)}) \end{array}$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 >=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 <=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	Е	12	42%	58%			
1	F	12	8	33%	17%		
1	G	12	25%	75%			
1	Н	12	58%	42%			

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Mol	Chain	Length	Qua	ality of chain
1	I	12	33%	67%
1	J	12	58%	42%
1	K	12	42%	58%
1	L	12	25%	75%
2	A	221	44%	51%
2	В	221	49%	48%
2	С	221	43%	52%
2	D	221	44%	48% 7% •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9396 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 RNA chain called 5'-R(*AP*AP*AP*UP*AP*UP*AP*UP*AP*UP*UP*U) -3'.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	Е	12	Total	С	N	О	Р	0	0	0
1	E	12	249	114	42	82	11	0	U	U
1	F	12	Total	С	N	О	Р	0	0	0
1	Г	12	249	114	42	82	11	0	U	0
1	G	12	Total	С	N	О	Р	0	0	0
1	G	12	249	114	42	82	11	0	U	
1	Н	12	Total	С	N	О	Р	0	0	0
1	11	12	249	114	42	82	11			0
1	I	12	Total	С	N	О	Р	0	0	0
1	1	12	249	114	42	82	11	0		
1	J	12	Total	С	N	О	Р	0	0	0
1	J	12	249	114	42	82	11	0	U	0
1	K	12	Total	С	N	О	Р	0	0	0
1		N 12	249	114	42	82	11	0	U	0
1	Т	12	Total	С	N	О	Р	0	0	0
1	1 L	12	249	114	42	82	11	0		U

• Molecule 2 is a protein called Ribonuclease III.

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
2	A 010		Total	С	N	О	S	0	0	0
2	A	219	1829	1191	306	331	1	U	U	0
2	В	219	Total	Total C N O S	0	0	0			
2	2 B	219	1829	1191	306	331	1	U	U	0
2	С	218	Total	С	N	О	S	0	0	0
2		210	1823	1188	305	329	1	0	U	U
2	D	219	Total	С	N	О	S	0	0	0
	ש	219	1829	1191	306	331	1	U	U	U

• Molecule 3 is water.



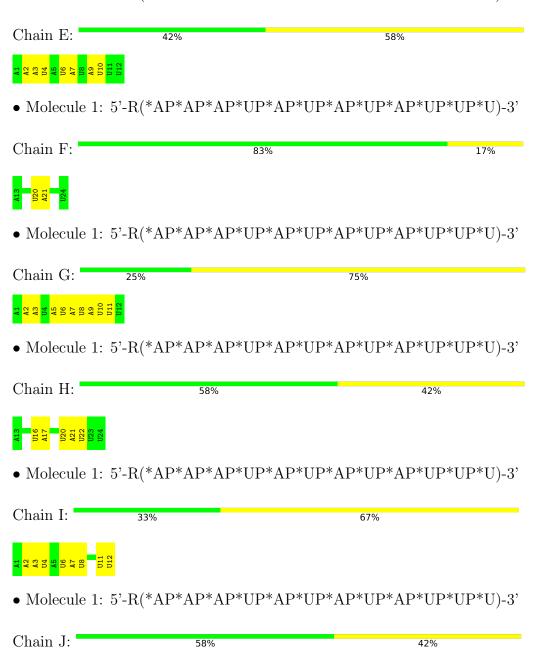
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Е	5	Total O 5 5	0	0
3	F	4	Total O 4 4	0	0
3	G	2	Total O 2 2	0	0
3	Н	3	Total O 3 3	0	0
3	I	2	Total O 2 2	0	0
3	К	1	Total O 1 1	0	0
3	L	3	Total O 3 3	0	0
3	A	26	Total O 26 26	0	0
3	В	19	Total O 19 19	0	0
3	С	12	Total O 12 12	0	0
3	D	17	Total O 17 17	0	0



3 Residue-property plots (i)

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: 5'-R(*AP*AP*AP*UP*AP*UP*AP*UP*AP*UP*UP*U)-3'







Chain K: 42% 58%

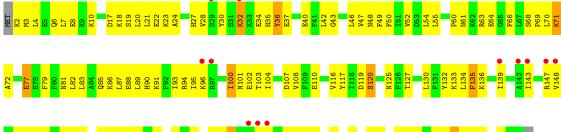
A1 A2 A3 U4 A5 A9 U10

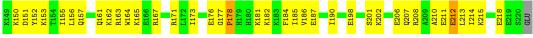
Chain L: 25% 75%

A13 U16 A17 U20 A21 U22 U22 U23

• Molecule 2: Ribonuclease III

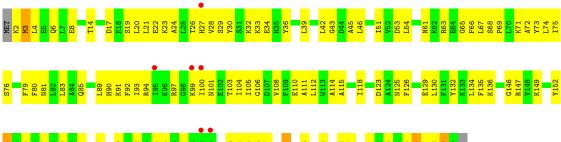
Chain A: 44% 51% .





• Molecule 2: Ribonuclease III

Chain B: 49% 48% ...

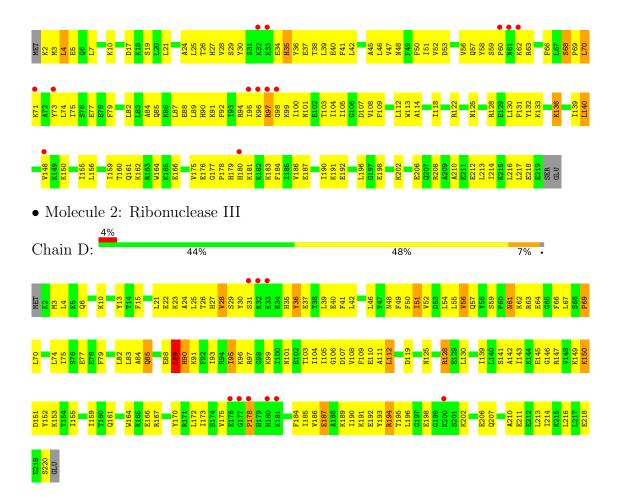


| 1158 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 | 1159 |

• Molecule 2: Ribonuclease III

Chain C: 43% 52% •







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	86.43Å 95.91Å 166.00Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 - 2.80	Depositor
Resolution (A)	29.98 - 2.70	EDS
% Data completeness	90.5 (29.98-2.80)	Depositor
(in resolution range)	83.3 (29.98-2.70)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.78 (at 2.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
D D.	0.243 , 0.314	Depositor
R, R_{free}	0.240 , 0.308	DCC
R_{free} test set	1920 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.28, 52.2	EDS
L-test for twinning ²	$ < L > = 0.46, < L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9396	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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 69.09 % 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 3.9226e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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	Во	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	Е	0.25	0/278	0.63	0/430		
1	F	0.21	0/278	0.64	0/430		
1	G	0.21	0/278	0.61	0/430		
1	Н	0.20	0/278	0.62	0/430		
1	I	0.24	0/278	0.62	0/430		
1	J	0.19	0/278	0.62	0/430		
1	K	0.22	0/278	0.64	0/430		
1	L	0.23	0/278	0.60	0/430		
2	A	0.36	0/1864	0.57	1/2493 (0.0%)		
2	В	0.30	0/1864	0.50	0/2493		
2	С	0.33	0/1858	0.53	0/2485		
2	D	0.41	0/1864	0.67	$2/2493 \ (0.1\%)$		
All	All	0.33	0/9674	0.58	3/13404 (0.0%)		

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	D	178	PRO	CA-N-CD	-10.06	97.42	111.50
2	A	178	PRO	CA-N-CD	-9.78	97.81	111.50
2	D	69	PRO	CA-N-CD	-7.45	101.07	111.50

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	Ε	249	0	128	6	0
1	F	249	0	128	1	0
1	G	249	0	128	8	0
1	Н	249	0	128	6	0
1	I	249	0	128	7	0
1	J	249	0	128	5	0
1	K	249	0	128	5	0
1	L	249	0	128	10	0
2	A	1829	0	1893	113	0
2	В	1829	0	1893	100	0
2	С	1823	0	1888	128	0
2	D	1829	0	1893	136	0
3	A	26	0	0	2	0
3	В	19	0	0	0	0
3	С	12	0	0	1	0
3	D	17	0	0	1	0
3	Е	5	0	0	0	0
3	F	4	0	0	0	0
3	G	2	0	0	0	0
3	Н	3	0	0	0	0
3	I	2	0	0	0	0
3	K	1	0	0	0	0
3	L	3	0	0	0	0
All	All	9396	0	8591	502	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 28.

The worst 5 of 502 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
2:C:41:PHE:CD2	2:D:67:LEU:HD13	1.85	1.12	
2:C:26:THR:CG2	2:C:94:ARG:HH21	1.71	1.03	
2:C:2:LYS:HG2	2:C:3:MET:H	1.24	1.00	
2:C:26:THR:HG21	2:C:94:ARG:HH21	1.30	0.94	
2:A:32:LYS:H	2:A:32:LYS:HD3	1.34	0.93	

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	Perce	entiles
2	A	217/221 (98%)	195 (90%)	20 (9%)	2 (1%)	17	46
2	В	217/221 (98%)	189 (87%)	26 (12%)	2 (1%)	17	46
2	С	216/221 (98%)	182 (84%)	29 (13%)	5 (2%)	6	21
2	D	217/221 (98%)	180 (83%)	30 (14%)	7 (3%)	4	13
All	All	867/884 (98%)	746 (86%)	105 (12%)	16 (2%)	8	28

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	135	PHE
2	С	60	PRO
2	D	90	HIS
2	В	46	LEU
2	В	216	LEU

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 Percent		ntiles	
2	A	196/198 (99%)	185 (94%)	11 (6%)		21	51
2	В	196/198 (99%)	188 (96%)	8 (4%)		30	64
2	С	195/198 (98%)	186 (95%)	9 (5%)		27	60
2	D	196/198 (99%)	179 (91%)	17 (9%)		10	30
All	All	783/792 (99%)	738 (94%)	45 (6%)		20	50



5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	3	MET
2	D	89	LEU
2	D	36	TYR
2	D	69	PRO
2	D	97	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	6	GLN
2	D	85	GLN
2	D	161	GLN
2	D	61	ASN
2	В	61	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Е	11/12 (91%)	0	0
1	F	11/12 (91%)	0	0
1	G	11/12 (91%)	0	0
1	Н	11/12 (91%)	0	0
1	I	11/12 (91%)	0	0
1	J	11/12 (91%)	0	0
1	K	11/12 (91%)	0	0
1	L	11/12 (91%)	0	0
All	All	88/96 (91%)	0	0

There are no RNA backbone outliers to report.

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 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 (i)

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^{th} 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>	#RSR2	Z>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	E	$12/12 \ (100\%)$	-0.46	0 100	100	32, 38, 50, 50	0
1	F	12/12 (100%)	-0.69	0 100	100	36, 47, 54, 56	0
1	G	12/12 (100%)	-0.57	0 100	100	39, 52, 58, 61	0
1	Н	12/12 (100%)	-0.48	0 100	100	30, 44, 60, 63	0
1	I	12/12 (100%)	-0.57	0 100	100	29, 40, 43, 49	0
1	J	12/12 (100%)	-0.76	0 100	100	34, 45, 53, 55	0
1	K	12/12 (100%)	-0.38	0 100	100	40, 51, 60, 64	0
1	L	12/12 (100%)	-0.53	0 100	100	32, 42, 57, 60	0
2	A	219/221 (99%)	0.04	12 (5%) 2	5 16	25, 61, 105, 117	0
2	В	219/221 (99%)	0.00	6 (2%) 54	44	25, 59, 98, 108	0
2	С	218/221 (98%)	0.32	13 (5%) 2	1 14	24, 74, 110, 119	0
2	D	219/221 (99%)	0.10	9 (4%) 37	7 27	26, 67, 103, 121	0
All	All	971/980 (99%)	0.05	40 (4%) 3'	7 27	24, 62, 105, 121	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	180	HIS	5.7
2	С	96	LYS	5.6
2	В	179	HIS	5.3
2	D	180	HIS	5.3
2	С	73	TYR	5.0

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 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.

