

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 21, 2023 – 06:01 AM JST

PDB ID	:	7F9N
Title	:	Crystal structure of the variable region of Plasmodium RIFIN $#4$
		$(PF3D7\_1000500)$ in complex with LAIR1
Authors	:	Xie, Y.; Song, H.; Li, X.; Qi, J.; Gao, G.F.
Deposited on	:	2021-07-04
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 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:

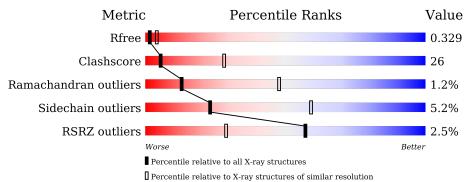
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)		
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	А	175	% 52%	34% •• 10%
1	В	175	% 54%	33% • 10%
2	С	112	% 54%	30% •• 12%
2	D	112	9%	<b>39%</b> • • 13%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3875 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	158	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	A		1169	730	207	226	6	0		
1	В	150	Total	С	Ν	Ο	S	0	0	0
1	В	B 158		730	207	226	6	0	0	0

• Molecule 1 is a protein called Rifin.

A149HIS-expression tagUNP A0A143ZWD5A150MET-expression tagUNP A0A143ZWD5A151HIS-expression tagUNP A0A143ZWD5A152HIS-expression tagUNP A0A143ZWD5A153HIS-expression tagUNP A0A143ZWD5A153HIS-expression tagUNP A0A143ZWD5A154HIS-expression tagUNP A0A143ZWD5A155HIS-expression tagUNP A0A143ZWD5A156HIS-expression tagUNP A0A143ZWD5B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5B156HIS-expression tagUNP A0A143ZWD5B156HIS-expression tagUNP A0A143ZWD5B156HIS-expres	Chain	Residue	Modelled	Actual	Comment	Reference
A151HIS-expression tagUNP A0A143ZWD5A152HIS-expression tagUNP A0A143ZWD5A153HIS-expression tagUNP A0A143ZWD5A154HIS-expression tagUNP A0A143ZWD5A155HIS-expression tagUNP A0A143ZWD5A155HIS-expression tagUNP A0A143ZWD5A156HIS-expression tagUNP A0A143ZWD5B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	A	149	HIS	-	expression tag	UNP A0A143ZWD5
A152HIS-expression tagUNP A0A143ZWD5A153HIS-expression tagUNP A0A143ZWD5A154HIS-expression tagUNP A0A143ZWD5A155HIS-expression tagUNP A0A143ZWD5A156HIS-expression tagUNP A0A143ZWD5B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	А	150	MET	-	expression tag	UNP A0A143ZWD5
A153HIS-expression tagUNP A0A143ZWD5A154HIS-expression tagUNP A0A143ZWD5A155HIS-expression tagUNP A0A143ZWD5A156HIS-expression tagUNP A0A143ZWD5B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	А	151	HIS	-	expression tag	UNP A0A143ZWD5
A154HIS-expression tagUNP A0A143ZWD5A155HIS-expression tagUNP A0A143ZWD5A156HIS-expression tagUNP A0A143ZWD5B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	А	152	HIS	-	expression tag	UNP A0A143ZWD5
A155HIS-expression tagUNP A0A143ZWD5A156HIS-expression tagUNP A0A143ZWD5B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	А	153	HIS	-	expression tag	UNP A0A143ZWD5
A156HIS-expression tagUNP A0A143ZWD5B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	А	154	HIS	-	expression tag	UNP A0A143ZWD5
B149HIS-expression tagUNP A0A143ZWD5B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	А	155	HIS	-	expression tag	UNP A0A143ZWD5
B150MET-expression tagUNP A0A143ZWD5B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	А	156	HIS	-	expression tag	UNP A0A143ZWD5
B151HIS-expression tagUNP A0A143ZWD5B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	В	149	HIS	-	expression tag	UNP A0A143ZWD5
B152HIS-expression tagUNP A0A143ZWD5B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	В	150	MET	-	expression tag	UNP A0A143ZWD5
B153HIS-expression tagUNP A0A143ZWD5B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	В	151	HIS	-	expression tag	UNP A0A143ZWD5
B154HIS-expression tagUNP A0A143ZWD5B155HIS-expression tagUNP A0A143ZWD5	В	152	HIS	-	expression tag	UNP A0A143ZWD5
B   155   HIS   -   expression tag   UNP A0A143ZWD5	В	153	HIS	-	expression tag	UNP A0A143ZWD5
	В	154	HIS	-	expression tag	UNP A0A143ZWD5
B156HIS-expression tagUNP A0A143ZWD5	В	155	HIS	-	expression tag	UNP A0A143ZWD5
	В	156	HIS	-	expression tag	UNP A0A143ZWD5

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Leukocyte-associated immunoglobulin-like receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	98	Total	С	Ν	0	S	0	0 0	0
			773	482	133	156	2	0		0
0	Л	07	Total	С	Ν	0	S	0	0	0
	2 D	97	764	477	132	153	2	0	0	0



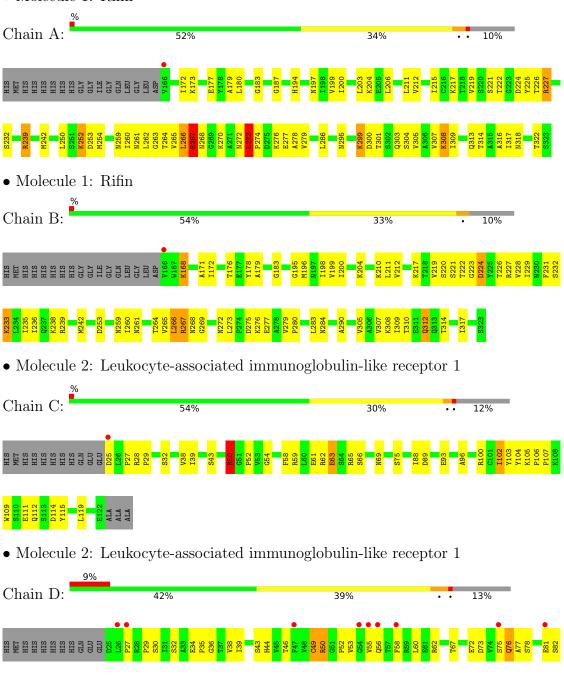
Chain	Residue	Modelled	Actual	Comment	Reference
С	14	HIS	-	expression tag	UNP Q6GTX8
С	15	MET	-	expression tag	UNP Q6GTX8
С	16	HIS	-	expression tag	UNP Q6GTX8
С	17	HIS	-	expression tag	UNP Q6GTX8
С	18	HIS	-	expression tag	UNP Q6GTX8
С	19	HIS	-	expression tag	UNP Q6GTX8
С	20	HIS	-	expression tag	UNP Q6GTX8
С	21	HIS	-	expression tag	UNP Q6GTX8
С	123	ALA	-	expression tag	UNP Q6GTX8
С	124	ALA	-	expression tag	UNP Q6GTX8
С	125	ALA	-	expression tag	UNP Q6GTX8
D	14	HIS	-	expression tag	UNP Q6GTX8
D	15	MET	-	expression tag	UNP Q6GTX8
D	16	HIS	-	expression tag	UNP Q6GTX8
D	17	HIS	-	expression tag	UNP Q6GTX8
D	18	HIS	-	expression tag	UNP Q6GTX8
D	19	HIS	-	expression tag	UNP Q6GTX8
D	20	HIS	-	expression tag	UNP Q6GTX8
D	21	HIS	-	expression tag	UNP Q6GTX8
D	123	ALA	-	expression tag	UNP Q6GTX8
D	124	ALA	-	expression tag	UNP Q6GTX8
D	125	ALA	-	expression tag	UNP Q6GTX8

There are 22 discrepancies between the modelled and reference sequences:



## 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: Rifin







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	73.44Å 73.44Å 341.05Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	49.67 - 3.00	Depositor
Resolution (A)	49.67 - 3.00	EDS
% Data completeness	99.6 (49.67-3.00)	Depositor
(in resolution range)	99.6 (49.67 - 3.00)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.14 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
D D.	0.264 , $0.330$	Depositor
$R, R_{free}$	0.264 , $0.329$	DCC
$R_{free}$ test set	996 reflections $(5.04\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	108.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , $72.3$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3875	wwPDB-VP
Average B, all atoms $(Å^2)$	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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	Boi	nd lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.52	0/1180	0.74	3/1596~(0.2%)	
1	В	0.43	0/1180	0.65	0/1596	
2	С	0.65	1/792~(0.1%)	0.98	6/1077~(0.6%)	
2	D	0.44	0/783	0.73	1/1065~(0.1%)	
All	All	0.51	1/3935~(0.0%)	0.77	10/5334~(0.2%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	50	ARG	CZ-NH2	5.56	1.40	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	50	ARG	NE-CZ-NH2	-12.39	114.10	120.30
2	С	50	ARG	NE-CZ-NH1	-11.05	114.78	120.30
2	С	50	ARG	NH1-CZ-NH2	8.43	128.68	119.40
1	А	266	LEU	CA-CB-CG	7.28	132.03	115.30
1	А	260	ILE	CG1-CB-CG2	-6.40	97.33	111.40

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	А	1169	0	1216	59	0
1	В	1169	0	1216	63	2
2	С	773	0	738	32	0
2	D	764	0	734	52	2
All	All	3875	0	3904	202	2

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 26.

The worst 5 of 202 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:D:100:ARG:NH2	2:D:115:TYR:CE2	2.05	1.22
2:D:100:ARG:NH2	2:D:115:TYR:HE2	1.42	1.16
2:C:102:ILE:HD11	2:C:112:GLN:HA	1.46	0.97
1:A:179:ALA:HA	1:A:309:ILE:HD11	1.44	0.97
2:C:32:SER:OG	2:C:50:ARG:NH1	1.98	0.96

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TYR:OH	2:D:100:ARG:NH1[6_464]	2.06	0.14
1:B:178:TYR:OH	2:D:100:ARG:NH2[6_464]	2.17	0.03

### 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
1	А	156/175~(89%)	138 (88%)	17 (11%)	1 (1%)	25	64
1	В	156/175~(89%)	142 (91%)	11 (7%)	3~(2%)	8	36

Continued on next page...



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	С	96/112~(86%)	89~(93%)	6~(6%)	1 (1%)	15 53
2	D	95/112~(85%)	88~(93%)	6~(6%)	1 (1%)	14 50
All	All	503/574 (88%)	457 (91%)	40 (8%)	6 (1%)	13 48

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5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	267	ARG
1	А	267	ARG
2	D	73	ASP
1	В	224	ASP
1	В	266	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	Percentiles
1	А	124/137~(90%)	116 (94%)	8~(6%)	17 50
1	В	124/137~(90%)	120~(97%)	4(3%)	39 74
2	С	88/99~(89%)	86~(98%)	2(2%)	50 80
2	D	87/99~(88%)	79~(91%)	8~(9%)	9 34
All	All	423/472~(90%)	401 (95%)	22~(5%)	23 59

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	32	SER
2	D	76	GLN
2	D	50	ARG
2	D	78	SER
1	А	304	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	214	ASN
1	А	272	ASN
1	В	192	ASN
1	В	312	GLN
2	С	112	GLN

#### 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 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>2	$OWAB(Å^2)$	Q<0.9
1	А	158/175~(90%)	-0.11	1 (0%) 89 72	80, 98, 119, 135	0
1	В	158/175~(90%)	-0.10	1 (0%) 89 72	99, 117, 134, 169	0
2	С	98/112~(87%)	-0.02	1 (1%) 82 59	78, 99, 129, 152	0
2	D	97/112~(86%)	0.66	10 (10%) 6 2	111, 154, 201, 221	0
All	All	511/574 (89%)	0.06	13 (2%) 57 29	78, 111, 171, 221	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	166	VAL	4.5
2	D	58	PHE	4.4
2	D	54	GLY	3.2
2	D	81	GLU	2.8
2	D	26	LEU	2.8

### 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.

