

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

#### Feb 13, 2025 – 10:06 AM EST

PDB ID	:	9DHU
Title	:	The Retinoblastoma Protein with Mutation E533K
Authors	:	Ruiz-Rivera, A.; Castro, A.; Burke, J.R.
Deposited on	:	2024-09-04
Resolution	:	2.16  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* 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

## 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 2.16 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	390	66%	19%	•	14%
1	В	390	4%	14%		• 9%



#### 9DHU

#### $\mathbf{2}$ Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11521 atoms, of which 5768 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 Retinoblastoma-associated protein.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
1	Δ	226	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
1	Π	000	5605	1793	2831	466	495	20	0	0	0
1	Р	252	Total	С	Η	Ν	0	S	0	0	0
	D	000	5842	1872	2937	488	524	21		U	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	377	GLY	-	expression tag	UNP P06400
А	378	GLU	-	expression tag	UNP P06400
А	379	PHE	-	expression tag	UNP P06400
А	533	LYS	GLU	conflict	UNP P06400
А	608	GLU	SER	conflict	UNP P06400
A	612	ALA	SER	conflict	UNP P06400
А	?	-	LYS	deletion	UNP P06400
А	?	-	GLY	deletion	UNP P06400
А	?	-	SER	deletion	UNP P06400
A	?	-	THR	deletion	UNP P06400
А	?	-	THR	deletion	UNP P06400
А	?	-	ARG	deletion	UNP P06400
А	?	-	VAL	deletion	UNP P06400
А	?	-	ASN	deletion	UNP P06400
А	?	-	SER	deletion	UNP P06400
А	?	-	THR	deletion	UNP P06400
А	?	-	ALA	deletion	UNP P06400
А	?	-	ASN	deletion	UNP P06400
А	?	-	ALA	deletion	UNP P06400
A	?	-	GLU	deletion	UNP P06400
А	?	-	THR	deletion	UNP P06400
А	?	-	GLN	deletion	UNP P06400
А	?	-	ALA	deletion	UNP P06400
А	?	-	THR	deletion	UNP P06400
А	?	-	SER	deletion	UNP P06400

There are 82 discrepancies between the modelled and reference sequences:



Continued from previous page							
Chain	Residue	Modelled	Actual	Comment	Reference		
А	?	-	ALA	deletion	UNP P06400		
А	?	-	PHE	deletion	UNP P06400		
А	?	-	GLN	deletion	UNP P06400		
А	?	-	THR	deletion	UNP P06400		
А	?	-	GLN	deletion	UNP P06400		
А	?	-	LYS	deletion	UNP P06400		
А	?	-	PRO	deletion	UNP P06400		
А	?	-	LEU	deletion	UNP P06400		
А	780	ALA	SER	conflict	UNP P06400		
А	787	PHE	-	expression tag	UNP P06400		
А	788	MET	-	expression tag	UNP P06400		
А	789	GLN	-	expression tag	UNP P06400		
А	790	ARG	-	expression tag	UNP P06400		
A	791	LEU	-	expression tag	UNP P06400		
А	792	LYS	-	expression tag	UNP P06400		
A	793	THR	_	expression tag	UNP P06400		
В	377	GLY	_	expression tag	UNP P06400		
В	378	GLU	-	expression tag	UNP P06400		
В	379	PHE	-	expression tag	UNP P06400		
В	533	LYS	GLU	conflict	UNP P06400		
В	608	GLU	SER	conflict	UNP P06400		
B	639	ALA	SER	conflict	UNP P06400		
B	?		LYS	deletion	UNP P06400		
B	?	_	GLY	deletion	UNP P06400		
В	?	_	SER	deletion	UNP P06400		
B	?	_	THR	deletion	UNP P06400		
B	?	_	THR	deletion	UNP P06400		
B	?	_	ARG	deletion	UNP P06400		
B	?		VAL	deletion	UNP P06400		
B	?		ASN	deletion	UNP P06400		
B	?		SER	deletion	UNP P06400		
B	. ?		THR	deletion	UNP P06400		
B	. ?		ALA	deletion	UNP P06400		
B	. ?		ASN	deletion	UNP P06400		
B	. ?			deletion	UNP P06400		
B	· · · · · · · · · · · · · · · · · · ·		GLU	deletion	UNP P06400		
B	?		THR	deletion	UNP P06400		
р В	2	-	CIN	deletion	UNI 100400		
D D	2	-		deletion	UNI 1 00400 UND D06400		
		-	ALA TUD	deletion	UNI FU0400		
		-	1 HK	deletion	UNP PU0400		
B		-	SER ALA	deletion	UNP P06400		
В		-	ALA	deletion	UNP P06400		



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Chain	Residue	Modelled	Actual	Comment	Reference
В	?	-	PHE	deletion	UNP P06400
В	?	-	GLN	deletion	UNP P06400
В	?	-	THR	deletion	UNP P06400
В	?	-	GLN	deletion	UNP P06400
В	?	-	LYS	deletion	UNP P06400
В	?	-	PRO	deletion	UNP P06400
В	?	-	LEU	deletion	UNP P06400
В	780	ALA	SER	conflict	UNP P06400
В	787	PHE	-	expression tag	UNP P06400
В	788	MET	-	expression tag	UNP P06400
В	789	GLN	-	expression tag	UNP P06400
В	790	ARG	-	expression tag	UNP P06400
В	791	LEU	-	expression tag	UNP P06400
B	792	LYS	-	expression tag	UNP P06400
В	793	THR	-	expression tag	UNP P06400

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	9	Total O 9 9	0	0
2	В	65	Total O 65 65	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: Retinoblastoma-associated protein



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	250.14Å $250.14$ Å $35.31$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	47.27 - 2.16	Depositor
Resolution (A)	47.27 - 2.16	EDS
% Data completeness	99.9 (47.27-2.16)	Depositor
(in resolution range)	99.9 (47.27-2.16)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 2.16 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
B B.	0.226 , $0.263$	Depositor
II, II, <i>free</i>	0.227 , $0.265$	DCC
$R_{free}$ test set	42183 reflections $(4.52%)$	wwPDB-VP
Wilson B-factor ( $Å^2$ )	38.6	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38 , $45.4$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11521	wwPDB-VP
Average B, all atoms $(Å^2)$	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.01% 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).

Mal	Chain	Bond lengths		Bond angles	
Moi Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.52	0/2829	0.72	0/3806
1	В	0.88	0/2964	0.89	0/3993
All	All	0.73	0/5793	0.81	0/7799

There are no bond length outliers.

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	А	2774	2831	2834	54	0
1	В	2905	2937	2955	36	0
2	А	9	0	0	0	0
2	В	65	0	0	2	0
All	All	5753	5768	5789	89	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 (89) 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:669:LEU:HD22	1:A:723:ILE:HG22	1.79	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:725:VAL:HG13	1:B:739:PHE:CZ	2.34	0.62
1:B:430:PHE:CE1	1:B:434:VAL:HG11	2.35	0.61
1:B:382:ILE:O	1:B:382:ILE:HG22	2.01	0.60
1:B:430:PHE:HE1	1:B:434:VAL:HG11	1.68	0.57
1:B:438:CYS:HB3	1:B:441:ILE:HD12	1.85	0.57
1:B:385:LEU:HB2	1:B:541:ASN:HB3	1.88	0.56
1:A:746:GLU:HA	1:A:746:GLU:OE1	2.05	0.56
1:B:600:HIS:CE1	2:B:804:HOH:O	2.58	0.56
1:A:461:LEU:HD11	1:A:477:LEU:HD21	1.86	0.56
1:A:698:ARG:NE	1:A:755:PHE:CE1	2.74	0.55
1:A:608:GLU:OE2	1:A:645:THR:N	2.38	0.54
1:B:546:MET:HE3	1:B:549:HIS:HB3	1.89	0.54
1:A:675:GLU:HG2	1:A:676:LEU:HD23	1.90	0.53
1:A:676:LEU:CD1	1:A:712:CYS:SG	2.97	0.53
1:B:449:GLY:HA3	1:B:491:LEU:HD23	1.91	0.52
1:A:556:ARG:HA	1:A:559:GLU:HG2	1.92	0.52
1:A:418:ARG:O	1:A:422:ILE:HG12	2.10	0.52
1:A:656:ARG:O	1:A:660:LEU:HG	2.10	0.52
1:A:449:GLY:HA3	1:A:491:LEU:HD23	1.91	0.51
1:A:398:GLU:O	1:A:401:ILE:HG13	2.11	0.51
1:A:712:CYS:HB3	1:A:717:ILE:HB	1.93	0.50
1:B:745:LYS:HE3	1:B:759:VAL:HG22	1.94	0.50
1:A:658:ALA:HB2	1:A:700:LEU:HD21	1.93	0.50
1:A:728:TYR:OH	1:A:738:THR:HG21	2.10	0.50
1:A:676:LEU:HD12	1:A:712:CYS:SG	2.53	0.49
1:A:491:LEU:O	1:A:495:MET:HG2	2.13	0.48
1:A:658:ALA:HB2	1:A:700:LEU:HD11	1.94	0.48
1:B:565:SER:O	1:B:566:ASP:HB2	2.12	0.48
1:B:557:ILE:HA	1:B:561:LEU:HB2	1.95	0.48
1:B:725:VAL:HG13	1:B:739:PHE:CE1	2.47	0.48
1:A:673:HIS:O	1:A:676:LEU:HG	2.13	0.48
1:A:720:LYS:HB2	1:A:722:LYS:HG2	1.95	0.48
1:A:658:ALA:HB1	1:A:684:PHE:CE2	2.49	0.47
1:A:714:VAL:HG11	1:A:768:ILE:HG22	1.96	0.47
1:A:430:PHE:CD2	1:A:442:GLY:CA	2.97	0.47
1:A:672:GLU:O	1:A:672:GLU:HG3	2.15	0.47
1:A:774:THR:HG1	1:B:511:ASP:N	2.13	0.47
1:A:453:TYR:HE2	1:A:454:TYR:CE1	2.33	0.46
1:A:642:LYS:HG3	1:A:643:LYS:N	2.30	0.46
1:B:516:TRP:CZ2	1:B:520:VAL:HG11	2.50	0.46
1:B:432:LYS:O	1:B:432:LYS:HD3	2.15	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:453:TYR:CE2	1:A:454:TYR:CE1	3.04	0.46
1:A:426:PHE:CD1	1:A:446:TYR:HB2	2.51	0.46
1:A:658:ALA:CA	1:A:700:LEU:HD21	2.46	0.45
1:B:411:PRO:HG3	1:B:477:LEU:HB3	1.97	0.45
1:A:411:PRO:HG3	1:A:477:LEU:HB3	1.99	0.45
1:B:668:ARG:HH11	1:B:668:ARG:CG	2.29	0.45
1:B:725:VAL:CG1	1:B:739:PHE:CE1	3.00	0.45
1:A:494:VAL:HG23	1:A:495:MET:N	2.32	0.45
1:A:517:ILE:HD11	1:A:521:LEU:HD11	1.99	0.45
1:B:438:CYS:O	1:B:441:ILE:N	2.46	0.44
1:B:470:ILE:HD12	1:B:470:ILE:H	1.83	0.44
1:B:423:GLY:O	1:B:427:LYS:HG3	2.18	0.44
1:B:491:LEU:O	1:B:495:MET:HG2	2.17	0.44
1:A:462:LYS:HD3	1:A:462:LYS:C	2.38	0.43
1:B:404:PHE:N	1:B:404:PHE:CD1	2.86	0.43
1:B:455:ARG:HG2	1:B:455:ARG:HH11	1.83	0.43
1:B:668:ARG:HH11	1:B:668:ARG:HG2	1.83	0.43
1:A:557:ILE:HA	1:A:561:LEU:HB2	2.00	0.43
1:B:445:ARG:NE	1:B:498:TYR:CD1	2.86	0.43
1:B:584:ASP:OD2	1:B:584:ASP:N	2.51	0.43
1:A:698:ARG:HG3	1:A:698:ARG:HH11	1.83	0.43
1:A:457:MET:O	1:A:461:LEU:HG	2.19	0.42
1:B:512:LEU:HD12	1:B:512:LEU:N	2.34	0.42
1:A:399:ASN:O	1:A:402:SER:OG	2.35	0.42
1:A:480:ASN:O	1:A:484:MET:HG2	2.20	0.42
1:B:426:PHE:CD1	1:B:446:TYR:HB2	2.53	0.42
1:B:475:LYS:O	1:B:476:LEU:C	2.57	0.42
1:A:758:SER:O	1:A:762:GLN:HG2	2.20	0.42
1:B:438:CYS:HB3	1:B:441:ILE:CD1	2.50	0.42
1:A:669:LEU:CD2	1:A:723:ILE:HG22	2.47	0.41
1:A:455:ARG:NH1	1:A:539:GLU:OE2	2.54	0.41
1:A:719:LEU:HD22	1:A:723:ILE:HD12	2.00	0.41
1:A:516:TRP:O	1:A:520:VAL:HG23	2.21	0.41
1:A:656:ARG:NH1	1:A:783:PRO:O	2.53	0.41
1:A:693:GLU:OE2	1:A:763:ARG:NH1	2.54	0.41
1:B:668:ARG:CG	1:B:668:ARG:NH1	2.84	0.41
1:A:516:TRP:CE2	1:A:520:VAL:CG2	3.04	0.41
1:B:392:ALA:O	1:B:451:ARG:NH1	2.41	0.41
1:A:611:ARG:HD3	1:A:611:ARG:HA	1.90	0.41
1:B:698:ARG:HA	2:B:840:HOH:O	2.21	0.41
1:A:466:GLU:O	1:A:466:GLU:HG3	2.22	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:TRP:CE2	1:A:520:VAL:HG21	2.57	0.40
1:A:747:GLU:O	1:A:747:GLU:CG	2.68	0.40
1:A:494:VAL:O	1:A:495:MET:C	2.60	0.40
1:A:513:SER:O	1:A:516:TRP:N	2.46	0.40
1:B:468:LEU:HB3	1:B:472:ASN:HB2	2.04	0.40
1:A:658:ALA:HA	1:A:700:LEU:HD21	2.04	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	А	326/390~(84%)	321 (98%)	5(2%)	0	100 100
1	В	345/390~(88%)	340 (99%)	5 (1%)	0	100 100
All	All	671/780~(86%)	661 (98%)	10 (2%)	0	100 100

There are no Ramachandran outliers to report.

#### 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	312/362~(86%)	302~(97%)	10 (3%)	34 34
1	В	328/362~(91%)	304~(93%)	24 (7%)	11 7



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	640/724~(88%)	606~(95%)	34~(5%)	19 16

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	397	SER
1	А	399	ASN
1	А	421	ASP
1	А	471	GLN
1	А	529	TYR
1	А	548	LYS
1	А	648	SER
1	А	698	ARG
1	А	747	GLU
1	А	766	THR
1	В	383	GLN
1	В	385	LEU
1	В	387	MET
1	В	402	SER
1	В	432	LYS
1	В	440	GLU
1	В	473	PHE
1	В	511	ASP
1	В	529	TYR
1	В	533	LYS
1	В	548	LYS
1	В	575	GLN
1	В	579	ARG
1	В	583	THR
1	В	584	ASP
1	В	600	HIS
1	В	608	GLU
1	В	668	ARG
1	В	713	LYS
1	В	714	VAL
1	В	725	VAL
1	В	747	GLU
1	В	748	GLU
1	В	775	ARG

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



#### 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 oligosaccharides 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	336/390~(86%)	1.06	40 (11%) 10 12	55, 95, 144, 183	0
1	В	353/390~(90%)	0.19	16 (4%) 39 44	23, 48, 92, 122	0
All	All	689/780~(88%)	0.61	56 (8%) 19 23	23, 72, 138, 183	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	612	ALA	4.5
1	В	610	VAL	4.0
1	В	383	GLN	3.9
1	А	724	ILE	3.8
1	В	382	ILE	3.7
1	В	437	GLY	3.6
1	А	761	MET	3.5
1	В	435	GLY	3.4
1	А	743	LEU	3.3
1	А	753	ILE	3.2
1	А	670	LEU	3.2
1	А	719	LEU	3.2
1	В	392	ALA	3.1
1	А	714	VAL	3.1
1	А	768	ILE	3.0
1	В	439	VAL	3.0
1	В	498	TYR	2.9
1	А	735	VAL	2.8
1	А	694	LEU	2.8
1	В	434	VAL	2.7
1	В	438	CYS	2.7
1	Α	600	HIS	2.6
1	А	760	PHE	2.6
1	A	782	ILE	2.6



9DHU		

Mol	Chain	Res	Type	RSRZ
1	А	749	TYR	2.6
1	А	723	ILE	2.6
1	А	717	ILE	2.6
1	А	499	SER	2.5
1	А	758	SER	2.4
1	А	728	TYR	2.4
1	А	755	PHE	2.4
1	А	733	HIS	2.3
1	В	387	MET	2.3
1	А	711	ILE	2.3
1	А	752	ILE	2.3
1	В	441	ILE	2.3
1	В	430	PHE	2.3
1	А	756	TYR	2.3
1	А	773	SER	2.2
1	А	669	LEU	2.2
1	В	541	ASN	2.2
1	В	385	LEU	2.2
1	А	424	TYR	2.2
1	В	388	ILE	2.1
1	А	665	LEU	2.1
1	А	544	ARG	2.1
1	А	401	ILE	2.1
1	А	571	ASP	2.1
1	А	772	ALA	2.1
1	А	732	PRO	2.1
1	А	779	LEU	2.1
1	A	425	ILE	2.1
1	А	575	GLN	2.0
1	А	731	LEU	2.0
1	А	441	ILE	2.0
1	А	394	ASP	2.0

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### 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.

