



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:40 AM GMT

PDB ID : 2DYL  
Title : Crystal structure of human mitogen-activated protein kinase kinase 7 activated mutant (S287D, T291D)  
Authors : Kukimoto-Niino, M.; Takagi, T.; Kaminishi, T.; Uchikubo-Kamo, T.; Terada, T.; Matsuzaki, O.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-09-15  
Resolution : 2.45 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



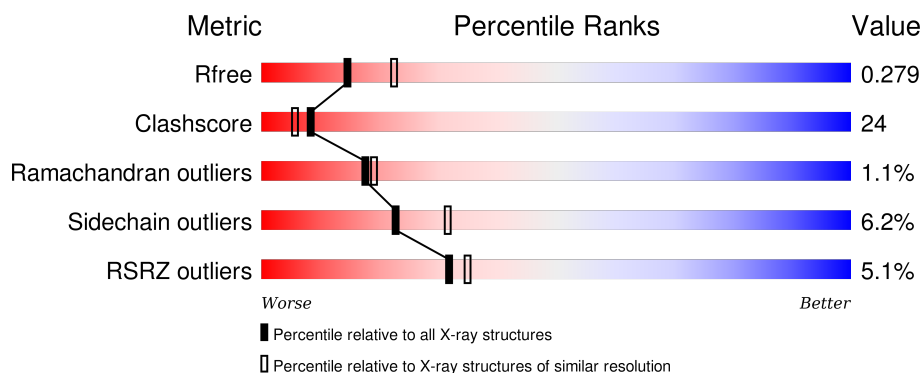
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	318	



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2233 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 Dual specificity mitogen-activated protein kinase kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2196	1404	378	396	18			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	GLY	-	EXPRESSION TAG	UNP O14733
A	111	SER	-	EXPRESSION TAG	UNP O14733
A	112	SER	-	EXPRESSION TAG	UNP O14733
A	113	GLY	-	EXPRESSION TAG	UNP O14733
A	114	SER	-	EXPRESSION TAG	UNP O14733
A	115	SER	-	EXPRESSION TAG	UNP O14733
A	116	GLY	-	EXPRESSION TAG	UNP O14733
A	287	ASP	SER	ENGINEERED	UNP O14733
A	291	ASP	THR	ENGINEERED	UNP O14733
A	422	SER	-	EXPRESSION TAG	UNP O14733
A	423	GLY	-	EXPRESSION TAG	UNP O14733
A	424	PRO	-	EXPRESSION TAG	UNP O14733
A	425	SER	-	EXPRESSION TAG	UNP O14733
A	426	SER	-	EXPRESSION TAG	UNP O14733
A	427	GLY	-	EXPRESSION TAG	UNP O14733

- Molecule 2 is water.

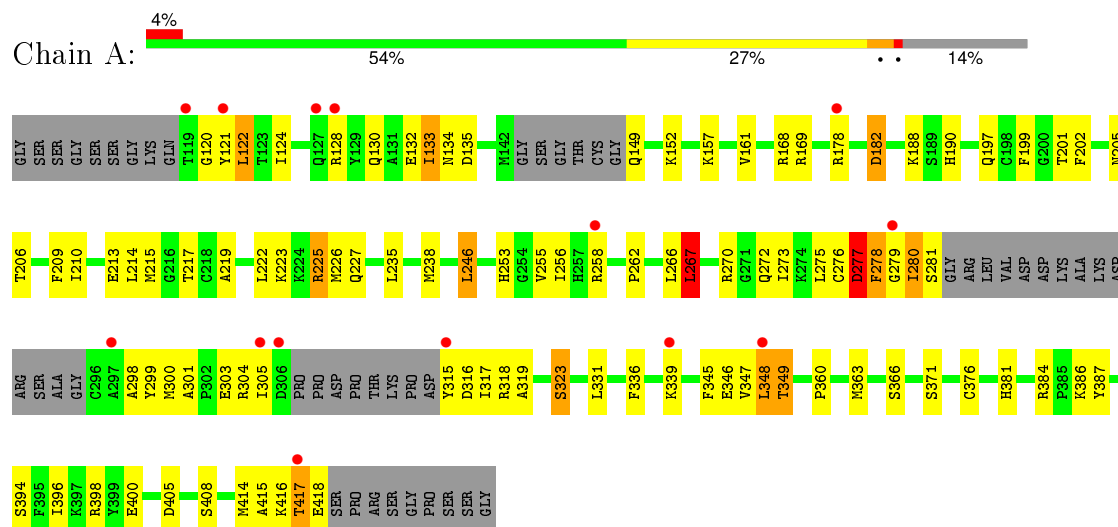
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		



### 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 errors 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: Dual specificity mitogen-activated protein kinase kinase 7





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.55Å 69.64Å 84.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.45 46.12 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.12-2.45) 98.9 (46.12-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.283 0.217 , 0.279	Depositor DCC
$R_{free}$ test set	1389 reflections (10.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 13677 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	0.48	0/2237	0.73	1/3003 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	CA-CB-CG	5.85	128.75	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2196	0	2231	107	0
2	A	37	0	0	2	0
All	All	2233	0	2231	107	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 24.

All (107) 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:258:ARG:HH22	1:A:319:ALA:HB3	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.26	0.99
1:A:278:PHE:CB	1:A:281:SER:HB3	1.99	0.92
1:A:152:LYS:HE3	1:A:161:VAL:HG11	1.54	0.87
1:A:278:PHE:HB3	1:A:281:SER:HB3	1.56	0.85
1:A:258:ARG:HA	1:A:258:ARG:HE	1.42	0.85
1:A:267:LEU:HD13	1:A:273:ILE:HG12	1.60	0.84
1:A:299:TYR:HB3	1:A:323:SER:HB3	1.62	0.80
1:A:255:VAL:HG11	1:A:281:SER:HB2	1.67	0.77
1:A:178:ARG:HD2	1:A:279:GLY:O	1.86	0.76
1:A:278:PHE:HB2	1:A:281:SER:HB3	1.67	0.75
1:A:258:ARG:NH2	1:A:319:ALA:HB3	1.96	0.74
1:A:415:ALA:C	1:A:417:THR:H	1.91	0.74
1:A:258:ARG:HA	1:A:258:ARG:NE	2.04	0.72
1:A:225:ARG:CG	1:A:225:ARG:HH11	2.00	0.72
1:A:298:ALA:HB1	1:A:336:PHE:CZ	2.26	0.71
1:A:278:PHE:HA	2:A:34:HOH:O	1.93	0.68
1:A:278:PHE:N	1:A:278:PHE:CD1	2.60	0.67
1:A:298:ALA:HB1	1:A:336:PHE:HZ	1.59	0.65
1:A:270:ARG:NH1	1:A:272:GLN:NE2	2.46	0.63
1:A:122:LEU:HD13	1:A:128:ARG:HH21	1.63	0.62
1:A:182:ASP:OD2	1:A:277:ASP:HA	2.00	0.61
1:A:122:LEU:HD22	1:A:130:GLN:OE1	2.00	0.61
1:A:225:ARG:CG	1:A:225:ARG:NH1	2.63	0.60
1:A:416:LYS:O	1:A:418:GLU:N	2.35	0.59
1:A:258:ARG:NH1	1:A:304:ARG:HD2	2.17	0.59
1:A:222:LEU:HD11	1:A:267:LEU:HG	1.84	0.59
1:A:396:ILE:O	1:A:400:GLU:HG3	2.02	0.59
1:A:300:MET:CE	1:A:305:ILE:HG12	2.32	0.58
1:A:190:HIS:HA	1:A:197:GLN:OE1	2.02	0.58
1:A:278:PHE:HB2	1:A:281:SER:CB	2.33	0.58
1:A:238:MET:HE1	1:A:331:LEU:CD1	2.34	0.58
1:A:225:ARG:HG3	1:A:225:ARG:NH1	2.06	0.57
1:A:415:ALA:C	1:A:417:THR:N	2.57	0.57
1:A:122:LEU:HD13	1:A:128:ARG:HE	1.69	0.56
1:A:256:ILE:O	1:A:258:ARG:HG2	2.05	0.56
1:A:255:VAL:CG1	1:A:281:SER:HB2	2.35	0.56
1:A:277:ASP:C	1:A:277:ASP:OD1	2.43	0.56
1:A:270:ARG:NH1	1:A:272:GLN:HE22	2.03	0.56
1:A:152:LYS:HE3	1:A:161:VAL:CG1	2.33	0.55
1:A:300:MET:HE2	1:A:305:ILE:HG12	1.88	0.55
1:A:124:ILE:HD11	1:A:128:ARG:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD13	1:A:128:ARG:NH2	2.22	0.55
1:A:417:THR:O	1:A:418:GLU:C	2.45	0.55
1:A:415:ALA:O	1:A:417:THR:HG22	2.07	0.54
1:A:258:ARG:CA	1:A:258:ARG:HE	2.15	0.54
1:A:303:GLU:OE1	1:A:381:HIS:HB3	2.08	0.54
1:A:258:ARG:HH12	1:A:304:ARG:HD2	1.73	0.53
1:A:238:MET:HE1	1:A:331:LEU:HD12	1.91	0.53
1:A:122:LEU:HD22	1:A:130:GLN:HE22	1.73	0.53
1:A:280:ILE:CG2	1:A:280:ILE:O	2.56	0.53
1:A:266:LEU:HD22	1:A:276:CYS:HB2	1.91	0.53
1:A:215:MET:HG3	1:A:266:LEU:HD23	1.90	0.52
1:A:316:ASP:OD1	1:A:318:ARG:HD3	2.09	0.52
1:A:366:SER:CB	1:A:398:ARG:HH22	2.22	0.52
1:A:188:LYS:HB3	1:A:253:HIS:CE1	2.44	0.52
1:A:258:ARG:HH22	1:A:319:ALA:CB	2.03	0.52
1:A:235:LEU:HD22	1:A:238:MET:HE1	1.92	0.52
1:A:149:GLN:HE21	1:A:168:ARG:HH21	1.57	0.52
1:A:149:GLN:NE2	1:A:168:ARG:HH21	2.08	0.51
1:A:122:LEU:HD22	1:A:130:GLN:NE2	2.26	0.51
1:A:416:LYS:C	1:A:418:GLU:N	2.63	0.51
1:A:298:ALA:HA	1:A:347:VAL:HG11	1.93	0.50
1:A:133:ILE:HG13	1:A:209:PHE:CE1	2.47	0.50
1:A:120:GLY:O	1:A:121:TYR:HB2	2.11	0.49
1:A:376:CYS:O	1:A:384:ARG:HD2	2.12	0.49
1:A:226:MET:O	1:A:227:GLN:HB2	2.12	0.49
1:A:280:ILE:HG22	1:A:280:ILE:O	2.13	0.48
1:A:122:LEU:HD13	1:A:128:ARG:NE	2.28	0.48
1:A:199:PHE:CZ	1:A:213:GLU:HB3	2.48	0.48
1:A:169:ARG:HD2	1:A:205:ASN:O	2.14	0.48
1:A:258:ARG:HD2	1:A:315:TYR:CE1	2.50	0.47
1:A:414:MET:HE2	1:A:414:MET:HA	1.97	0.47
1:A:316:ASP:N	1:A:316:ASP:OD2	2.48	0.46
1:A:222:LEU:CD1	1:A:267:LEU:HG	2.46	0.46
1:A:223:LYS:HG3	2:A:29:HOH:O	2.15	0.46
1:A:121:TYR:C	1:A:122:LEU:HD23	2.36	0.46
1:A:121:TYR:O	1:A:122:LEU:HD23	2.16	0.46
1:A:345:PHE:HA	1:A:348:LEU:CD2	2.46	0.45
1:A:416:LYS:O	1:A:417:THR:C	2.54	0.45
1:A:301:ALA:O	1:A:305:ILE:HG13	2.16	0.44
1:A:238:MET:CE	1:A:331:LEU:HD12	2.47	0.44
1:A:149:GLN:NE2	1:A:168:ARG:NH2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:C	1:A:280:ILE:H	2.21	0.44
1:A:303:GLU:CD	1:A:384:ARG:HH22	2.21	0.43
1:A:303:GLU:OE1	1:A:384:ARG:NH2	2.43	0.43
1:A:219:ALA:HB3	1:A:262:PRO:O	2.18	0.43
1:A:414:MET:CE	1:A:414:MET:HA	2.49	0.43
1:A:300:MET:HE3	1:A:305:ILE:HG12	1.99	0.43
1:A:360:PRO:HG2	1:A:363:MET:CE	2.48	0.43
1:A:345:PHE:HA	1:A:348:LEU:HD23	2.00	0.43
1:A:152:LYS:CE	1:A:161:VAL:HG11	2.38	0.42
1:A:135:ASP:OD1	1:A:157:LYS:HE3	2.19	0.42
1:A:161:VAL:HG12	1:A:214:LEU:HD22	2.00	0.42
1:A:122:LEU:HD22	1:A:130:GLN:CD	2.39	0.42
1:A:238:MET:HE1	1:A:331:LEU:HD13	2.02	0.41
1:A:246:LEU:CD1	1:A:275:LEU:HD11	2.50	0.41
1:A:201:THR:CG2	1:A:202:PHE:N	2.82	0.41
1:A:132:GLU:HG3	1:A:134:ASN:H	1.85	0.41
1:A:346:GLU:O	1:A:349:THR:HB	2.20	0.41
1:A:317:ILE:HD11	1:A:386:LYS:HG2	2.03	0.41
1:A:210:ILE:N	1:A:210:ILE:HD12	2.36	0.40
1:A:235:LEU:HD22	1:A:238:MET:CE	2.51	0.40
1:A:316:ASP:OD1	1:A:318:ARG:NH1	2.54	0.40
1:A:317:ILE:HB	1:A:387:TYR:CE1	2.57	0.40
1:A:169:ARG:CD	1:A:206:THR:HA	2.51	0.40
1:A:405:ASP:OD2	1:A:408:SER:OG	2.35	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	264/318 (83%)	248 (94%)	13 (5%)	3 (1%)	17 19



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASP
1	A	417	THR
1	A	280	ILE

### 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	241/275 (88%)	226 (94%)	15 (6%)	23	31

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	133	ILE
1	A	182	ASP
1	A	217	THR
1	A	225	ARG
1	A	246	LEU
1	A	267	LEU
1	A	277	ASP
1	A	278	PHE
1	A	323	SER
1	A	339	LYS
1	A	348	LEU
1	A	349	THR
1	A	371	SER
1	A	394	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	272	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 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 [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<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	272/318 (85%)	0.29	14 (5%) 32 35	26, 43, 72, 99	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	TYR	4.9
1	A	121	TYR	3.4
1	A	258	ARG	3.2
1	A	305	ILE	2.8
1	A	339	LYS	2.7
1	A	279	GLY	2.6
1	A	128	ARG	2.6
1	A	306	ASP	2.5
1	A	297	ALA	2.5
1	A	178	ARG	2.2
1	A	127	GLN	2.2
1	A	348	LEU	2.2
1	A	119	THR	2.1
1	A	417	THR	2.1

### 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.