



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:25 PM GMT

PDB ID : 3ZFW  
Title : Crystal structure of the TPR domain of kinesin light chain 2 in complex with a tryptophan-acidic cargo peptide  
Authors : Pernigo, S.; Lamprecht, A.; Steiner, R.A.; Dodding, M.P.  
Deposited on : 2012-12-12  
Resolution : 2.90 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

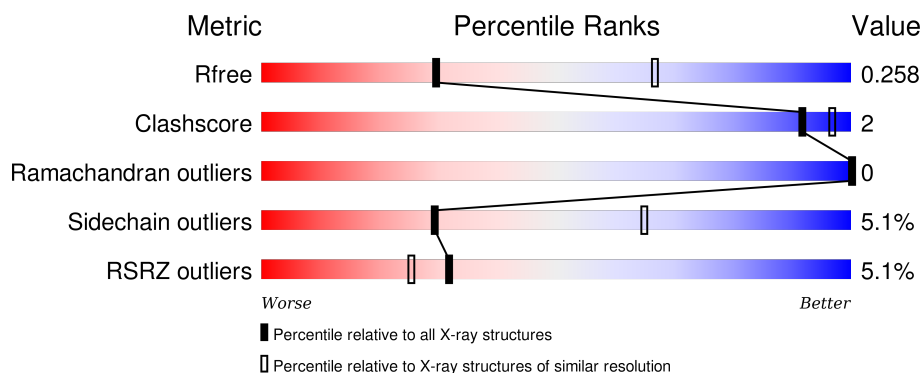
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	263	<div> <div>4%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
1	B	263	<div> <div>4%</div> <div>77%</div> <div>8%</div> <div>14%</div> </div>
2	X	45	<div> <div>4%</div> <div>22%</div> <div>76%</div> </div>
2	Y	45	<div> <div>4%</div> <div>20%</div> <div>78%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3749 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 KINESIN LIGHT CHAIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1794	1121	327	339	7			
1	B	225	Total	C	N	O	S	0	0	0
			1786	1118	324	337	7			

- Molecule 2 is a protein called PLECKSTRIN HOMOLOGY DOMAIN-CONTAINING FAMILY M MEMBER 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	11	Total	C	N	O	0	0	0
			88	54	13	21			
2	Y	10	Total	C	N	O	0	0	0
			81	50	12	19			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	182	MET	-	EXPRESSION TAG	UNP Q81WE5
X	183	GLY	-	EXPRESSION TAG	UNP Q81WE5
X	184	SER	-	EXPRESSION TAG	UNP Q81WE5
X	185	SER	-	EXPRESSION TAG	UNP Q81WE5
X	186	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	187	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	188	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	189	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	190	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	191	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	192	SER	-	EXPRESSION TAG	UNP Q81WE5
X	193	SER	-	EXPRESSION TAG	UNP Q81WE5
X	194	GLY	-	EXPRESSION TAG	UNP Q81WE5
X	195	LEU	-	EXPRESSION TAG	UNP Q81WE5
X	196	VAL	-	EXPRESSION TAG	UNP Q81WE5
X	197	PRO	-	EXPRESSION TAG	UNP Q81WE5

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Chain	Residue	Modelled	Actual	Comment	Reference
X	198	ARG	-	EXPRESSION TAG	UNP Q81WE5
X	199	GLY	-	EXPRESSION TAG	UNP Q81WE5
X	200	SER	-	EXPRESSION TAG	UNP Q81WE5
X	201	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	202	MET	-	EXPRESSION TAG	UNP Q81WE5
X	213	THR	-	EXPRESSION TAG	UNP Q81WE5
X	214	GLY	-	EXPRESSION TAG	UNP Q81WE5
X	215	SER	-	EXPRESSION TAG	UNP Q81WE5
X	216	THR	-	EXPRESSION TAG	UNP Q81WE5
X	217	GLY	-	EXPRESSION TAG	UNP Q81WE5
X	218	SER	-	EXPRESSION TAG	UNP Q81WE5
X	219	THR	-	EXPRESSION TAG	UNP Q81WE5
X	220	GLY	-	EXPRESSION TAG	UNP Q81WE5
X	221	SER	-	EXPRESSION TAG	UNP Q81WE5
X	222	THR	-	EXPRESSION TAG	UNP Q81WE5
X	223	GLY	-	EXPRESSION TAG	UNP Q81WE5
X	224	SER	-	EXPRESSION TAG	UNP Q81WE5
X	225	HIS	-	EXPRESSION TAG	UNP Q81WE5
X	226	MET	-	EXPRESSION TAG	UNP Q81WE5
Y	182	MET	-	EXPRESSION TAG	UNP Q81WE5
Y	183	GLY	-	EXPRESSION TAG	UNP Q81WE5
Y	184	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	185	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	186	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	187	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	188	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	189	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	190	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	191	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	192	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	193	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	194	GLY	-	EXPRESSION TAG	UNP Q81WE5
Y	195	LEU	-	EXPRESSION TAG	UNP Q81WE5
Y	196	VAL	-	EXPRESSION TAG	UNP Q81WE5
Y	197	PRO	-	EXPRESSION TAG	UNP Q81WE5
Y	198	ARG	-	EXPRESSION TAG	UNP Q81WE5
Y	199	GLY	-	EXPRESSION TAG	UNP Q81WE5
Y	200	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	201	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	202	MET	-	EXPRESSION TAG	UNP Q81WE5
Y	213	THR	-	EXPRESSION TAG	UNP Q81WE5
Y	214	GLY	-	EXPRESSION TAG	UNP Q81WE5

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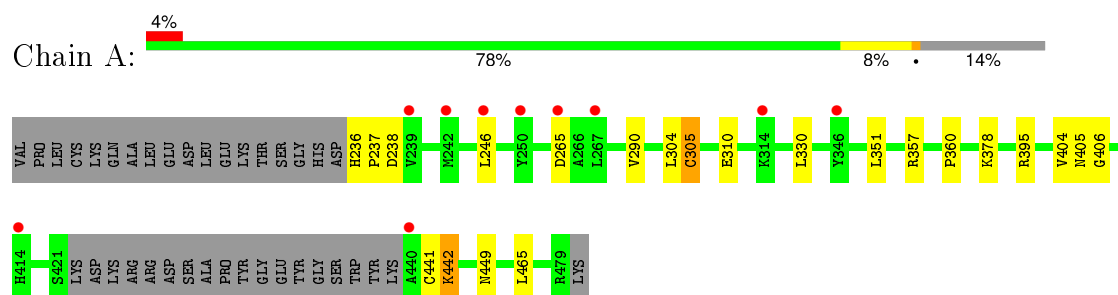
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Chain	Residue	Modelled	Actual	Comment	Reference
Y	215	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	216	THR	-	EXPRESSION TAG	UNP Q81WE5
Y	217	GLY	-	EXPRESSION TAG	UNP Q81WE5
Y	218	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	219	THR	-	EXPRESSION TAG	UNP Q81WE5
Y	220	GLY	-	EXPRESSION TAG	UNP Q81WE5
Y	221	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	222	THR	-	EXPRESSION TAG	UNP Q81WE5
Y	223	GLY	-	EXPRESSION TAG	UNP Q81WE5
Y	224	SER	-	EXPRESSION TAG	UNP Q81WE5
Y	225	HIS	-	EXPRESSION TAG	UNP Q81WE5
Y	226	MET	-	EXPRESSION TAG	UNP Q81WE5

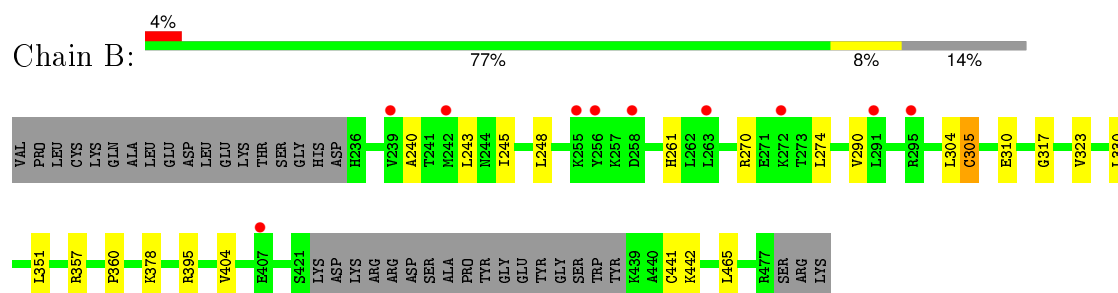
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

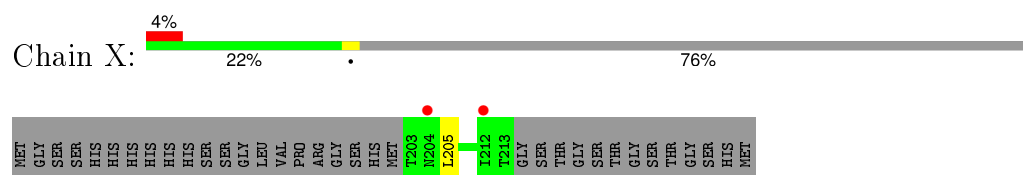
#### • Molecule 1: KINESIN LIGHT CHAIN 2



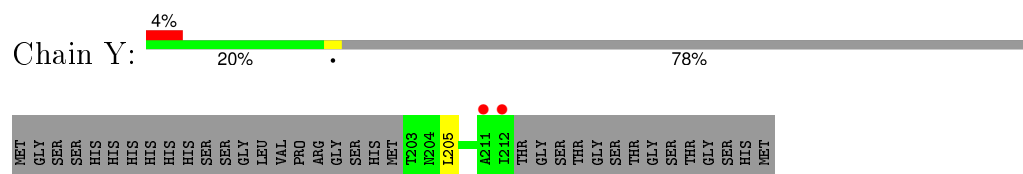
#### • Molecule 1: KINESIN LIGHT CHAIN 2



#### • Molecule 2: PLECKSTRIN HOMOLOGY DOMAIN-CONTAINING FAMILY M MEMBER 2



#### • Molecule 2: PLECKSTRIN HOMOLOGY DOMAIN-CONTAINING FAMILY M MEMBER 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.81Å 90.86Å 94.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.42 – 2.90 52.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (52.42-2.90) 98.7 (52.42-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.202 , 0.244 0.216 , 0.258	Depositor DCC
$R_{free}$ test set	854 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 77.1	EDS
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17031 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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 [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	0.46	0/1823	0.62	0/2457
1	B	0.46	0/1815	0.62	0/2446
2	X	0.49	0/89	0.67	0/122
2	Y	0.48	0/82	0.73	0/112
All	All	0.46	0/3809	0.62	0/5137

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	A	1794	0	1804	8	0
1	B	1786	0	1799	9	0
2	X	88	0	75	1	0
2	Y	81	0	68	1	0
All	All	3749	0	3746	16	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 2.

All (16) 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:246:LEU:HD21	1:B:243:LEU:HD23	1.71	0.73
1:A:305:CYS:HB3	1:A:330:LEU:HD13	1.82	0.60
1:B:305:CYS:HB3	1:B:330:LEU:HD13	1.82	0.60
1:B:240:ALA:HA	1:B:243:LEU:HD12	1.91	0.52
1:A:290:VAL:HG22	2:X:205:LEU:HB3	1.91	0.52
1:B:290:VAL:HG22	2:Y:205:LEU:HB3	1.92	0.51
1:A:405:ASN:HD22	1:A:406:GLY:H	1.61	0.48
1:B:441:CYS:SG	1:B:442:LYS:N	2.85	0.46
1:A:360:PRO:HB2	1:A:395:ARG:HD3	1.97	0.46
1:A:236:HIS:CD2	1:A:238:ASP:H	2.34	0.45
1:A:441:CYS:SG	1:A:442:LYS:N	2.89	0.45
1:B:270:ARG:HG2	1:B:274:LEU:HD12	2.00	0.44
1:B:360:PRO:HB2	1:B:395:ARG:HD3	1.99	0.44
1:B:245:ILE:HA	1:B:248:LEU:HD12	1.98	0.43
1:A:236:HIS:ND1	1:A:237:PRO:HD2	2.35	0.42
1:B:317:GLY:O	1:B:323:VAL:HG21	2.21	0.41

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	222/263 (84%)	210 (95%)	12 (5%)	0	100	100
1	B	221/263 (84%)	207 (94%)	14 (6%)	0	100	100
2	X	9/45 (20%)	9 (100%)	0	0	100	100
2	Y	8/45 (18%)	8 (100%)	0	0	100	100
All	All	460/616 (75%)	434 (94%)	26 (6%)	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	188/220 (86%)	177 (94%)	11 (6%)	24	58
1	B	187/220 (85%)	178 (95%)	9 (5%)	31	67
2	X	10/37 (27%)	10 (100%)	0	100	100
2	Y	9/37 (24%)	9 (100%)	0	100	100
All	All	394/514 (77%)	374 (95%)	20 (5%)	29	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	A	304	LEU
1	A	305	CYS
1	A	310	GLU
1	A	351	LEU
1	A	357	ARG
1	A	378	LYS
1	A	404	VAL
1	A	442	LYS
1	A	449	ASN
1	A	465	LEU
1	B	261	HIS
1	B	304	LEU
1	B	305	CYS
1	B	310	GLU
1	B	351	LEU
1	B	357	ARG
1	B	378	LYS
1	B	404	VAL
1	B	465	LEU

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

Mol	Chain	Res	Type
1	A	244	ASN
1	A	405	ASN
1	A	408	ASN
1	B	405	ASN
1	B	408	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	226/263 (85%)	0.56	10 (4%) 38 32	57, 111, 147, 170	0
1	B	225/263 (85%)	0.56	10 (4%) 38 32	59, 109, 149, 165	0
2	X	11/45 (24%)	0.72	2 (18%) 2 1	101, 128, 152, 163	0
2	Y	10/45 (22%)	1.13	2 (20%) 1 1	108, 125, 136, 173	0
All	All	472/616 (76%)	0.57	24 (5%) 32 25	57, 111, 149, 173	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	212	ILE	7.1
1	A	440	ALA	4.1
1	B	407	GLU	3.9
1	A	242	MET	3.6
1	B	242	MET	3.5
1	A	265	ASP	3.3
1	B	256	TYR	3.3
1	B	239	VAL	3.3
1	B	258	ASP	3.1
2	Y	211	ALA	3.0
1	A	239	VAL	2.9
1	A	250	TYR	2.9
1	B	295	ARG	2.9
1	A	246	LEU	2.7
1	B	272	LYS	2.6
1	A	314	LYS	2.4
2	X	212	ILE	2.4
1	B	255	LYS	2.3
2	X	204	ASN	2.3
1	A	414	HIS	2.2
1	A	346	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	291	LEU	2.0
1	B	263	LEU	2.0
1	A	267	LEU	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.