



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:22 PM GMT

PDB ID : 2WZJ  
Title : CATALYTIC AND UBA DOMAIN OF KINASE MARK2/(PAR-1) K82R,  
T208E DOUBLE MUTANT  
Authors : Panneerselvam, S.; Marx, A.; Mandelkow, E.-M.; Mandelkow, E.  
Deposited on : 2009-11-30  
Resolution : 2.79 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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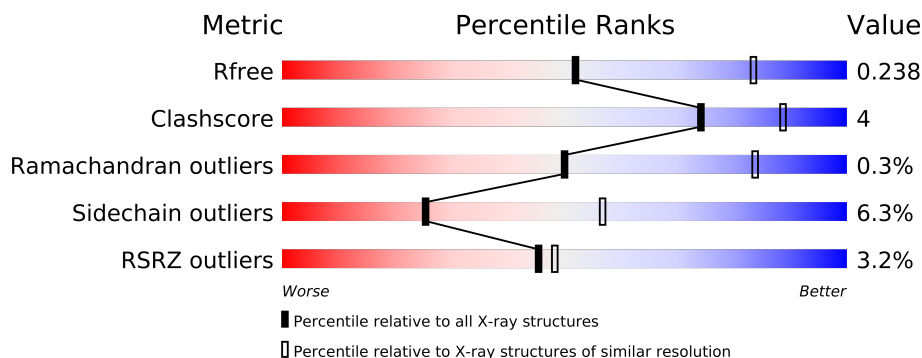
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.79 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))
$R_{free}$	66092	2193 (2.80-2.76)
Clashscore	79885	2751 (2.80-2.76)
Ramachandran outliers	78287	2699 (2.80-2.76)
Sidechain outliers	78261	2701 (2.80-2.76)
RSRZ outliers	66119	2196 (2.80-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	
1	C	327	
1	D	327	
1	E	327	
1	F	327	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15326 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SERINE/THREONINE-PROTEINKINASE MARK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2531	1627	432	459	13			
1	B	310	Total	C	N	O	S	0	0	0
			2531	1627	432	459	13			
1	C	310	Total	C	N	O	S	0	0	0
			2531	1627	432	459	13			
1	D	313	Total	C	N	O	S	0	0	0
			2556	1642	436	465	13			
1	E	310	Total	C	N	O	S	0	0	0
			2531	1627	432	459	13			
1	F	310	Total	C	N	O	S	0	0	0
			2531	1627	432	459	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ARG	LYS	ENGINEERED MUTATION	UNP O08679
A	208	GLU	THR	ENGINEERED MUTATION	UNP O08679
B	82	ARG	LYS	ENGINEERED MUTATION	UNP O08679
B	208	GLU	THR	ENGINEERED MUTATION	UNP O08679
C	82	ARG	LYS	ENGINEERED MUTATION	UNP O08679
C	208	GLU	THR	ENGINEERED MUTATION	UNP O08679
D	82	ARG	LYS	ENGINEERED MUTATION	UNP O08679
D	208	GLU	THR	ENGINEERED MUTATION	UNP O08679
E	82	ARG	LYS	ENGINEERED MUTATION	UNP O08679
E	208	GLU	THR	ENGINEERED MUTATION	UNP O08679
F	82	ARG	LYS	ENGINEERED MUTATION	UNP O08679
F	208	GLU	THR	ENGINEERED MUTATION	UNP O08679

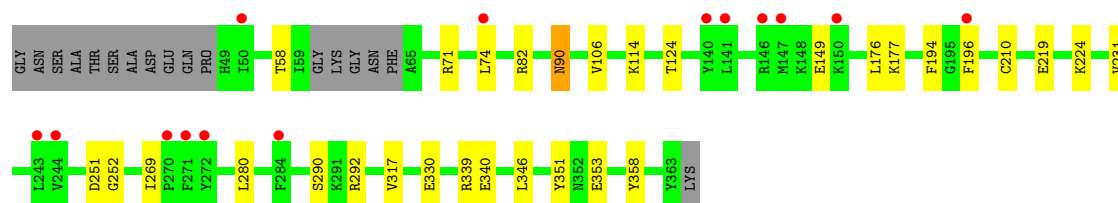
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total 36	O 36	0	0
2	B	31	Total 31	O 31	0	0
2	C	13	Total 13	O 13	0	0
2	D	24	Total 24	O 24	0	0
2	E	3	Total 3	O 3	0	0
2	F	8	Total 8	O 8	0	0



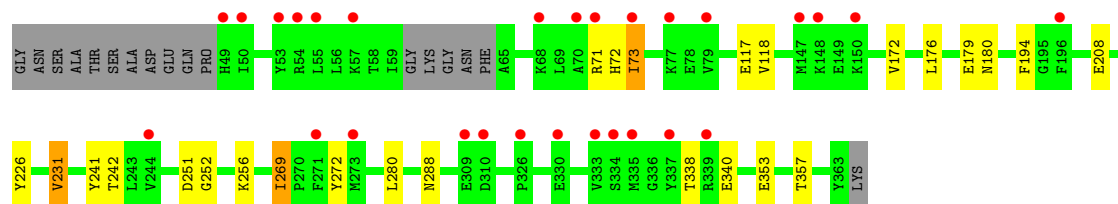
• Molecule 1: SERINE/THREONINE-PROTEINKINASE MARK2

Chain E:



• Molecule 1: SERINE/THREONINE-PROTEINKINASE MARK2

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.24Å 205.58Å 91.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.39 – 2.79 45.39 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.39-2.79) 99.6 (45.39-2.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.179 , 0.246 0.171 , 0.238	Depositor DCC
$R_{free}$ test set	3846 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 76697 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.46	0/2582	0.59	0/3476
1	B	0.44	0/2582	0.62	0/3476
1	C	0.42	0/2582	0.57	0/3476
1	D	0.42	0/2608	0.60	0/3512
1	E	0.35	0/2582	0.52	0/3476
1	F	0.35	0/2582	0.51	0/3476
All	All	0.41	0/15518	0.57	0/20892

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2531	0	0	8	0
1	B	2531	0	0	10	0
1	C	2531	0	0	8	0
1	D	2556	0	0	21	0
1	E	2531	0	0	8	0
1	F	2531	0	0	9	0
2	A	36	0	0	1	0
2	B	31	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	0	0	0
2	D	24	0	0	4	0
2	E	3	0	0	0	0
2	F	8	0	0	1	0
All	All	15326	0	0	62	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (62) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:57:LYS:NZ	2:D:2004:HOH:O	2.30	0.65
1:A:90:ASN:N	1:A:90:ASN:ND2	2.48	0.61
1:D:196:PHE:CE1	1:D:202:PHE:CZ	2.90	0.59
1:D:339:ARG:NE	2:D:2021:HOH:O	2.37	0.58
1:D:288:ASN:ND2	1:D:288:ASN:C	2.57	0.58
1:F:251:ASP:OD1	1:F:252:GLY:N	2.38	0.57
1:B:288:ASN:ND2	1:B:288:ASN:C	2.58	0.56
1:D:219:GLU:OE2	1:D:292:ARG:NH2	2.39	0.54
1:D:196:PHE:CE1	1:D:202:PHE:CE2	2.95	0.54
1:B:53:TYR:OH	1:B:117:GLU:OE1	2.27	0.53
1:D:57:LYS:CE	2:D:2004:HOH:O	2.58	0.51
1:F:72:HIS:O	1:F:73:ILE:C	2.49	0.51
1:D:58:THR:CG2	1:D:68:LYS:NZ	2.74	0.50
1:F:357:THR:N	2:F:2008:HOH:O	2.44	0.50
1:B:200:PHE:CD1	1:B:201:THR:O	2.66	0.49
1:C:104:MET:CE	1:C:196:PHE:CD2	2.95	0.49
1:C:226:TYR:CE1	1:C:231:VAL:CG1	2.96	0.49
1:A:177:LYS:NZ	1:A:199:GLU:OE1	2.47	0.48
1:E:177:LYS:NZ	1:E:210:CYS:O	2.46	0.48
1:A:104:MET:CE	1:A:196:PHE:CB	2.92	0.48
1:C:90:ASN:ND2	1:C:90:ASN:N	2.62	0.48
1:F:179:GLU:N	1:F:179:GLU:OE1	2.47	0.47
1:D:310:ASP:OD1	1:D:310:ASP:N	2.47	0.47
1:D:226:TYR:CE1	1:D:231:VAL:CG1	2.98	0.47
1:F:226:TYR:CE1	1:F:231:VAL:CG1	2.98	0.47
1:D:238:VAL:O	1:D:242:THR:CG2	2.62	0.47
1:C:311:ASP:O	1:C:312:GLU:C	2.53	0.47
1:B:90:ASN:ND2	1:B:90:ASN:N	2.63	0.47
1:E:251:ASP:OD1	1:E:252:GLY:N	2.48	0.47
1:D:271:PHE:CD2	1:D:271:PHE:N	2.83	0.46
1:D:341:GLU:CD	2:D:2022:HOH:O	2.55	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:230:GLU:OE1	1:C:230:GLU:N	2.50	0.45
1:D:184:ASP:OD1	1:D:184:ASP:C	2.55	0.45
1:C:173:HIS:N	1:C:232:ASP:OD2	2.50	0.45
1:E:330:GLU:OE1	1:E:339:ARG:NH2	2.50	0.45
1:F:269:ILE:N	1:F:269:ILE:CD1	2.80	0.44
1:E:82:ARG:NE	1:E:196:PHE:CZ	2.85	0.44
1:B:227:ASP:N	2:B:2020:HOH:O	2.50	0.44
1:D:96:LYS:NZ	1:D:100:GLU:OE2	2.50	0.44
1:D:200:PHE:CG	1:D:200:PHE:O	2.71	0.44
1:E:346:LEU:CD1	1:E:358:TYR:CD1	3.00	0.44
1:A:148:LYS:N	2:A:2011:HOH:O	2.49	0.43
1:D:90:ASN:O	1:D:93:SER:N	2.51	0.43
1:F:241:TYR:CD1	1:F:241:TYR:O	2.72	0.43
1:E:90:ASN:ND2	1:E:90:ASN:N	2.67	0.43
1:E:114:LYS:NZ	1:E:351:TYR:OH	2.51	0.43
1:B:148:LYS:N	2:B:2008:HOH:O	2.51	0.43
1:A:179:GLU:OE2	1:F:208:GLU:OE2	2.36	0.43
1:B:228:GLY:N	2:B:2020:HOH:O	2.51	0.43
1:D:346:LEU:O	1:D:349:GLN:NE2	2.53	0.42
1:B:90:ASN:ND2	1:B:93:SER:OG	2.52	0.42
1:E:219:GLU:OE2	1:E:292:ARG:NH2	2.52	0.42
1:A:219:GLU:OE2	1:A:292:ARG:NH2	2.52	0.42
1:D:82:ARG:NE	1:D:196:PHE:CE2	2.87	0.42
1:D:338:THR:O	1:D:342:ILE:CG1	2.68	0.42
1:B:82:ARG:NE	1:B:196:PHE:CZ	2.88	0.42
1:C:272:TYR:CD1	1:C:273:MET:N	2.88	0.41
1:A:288:ASN:C	1:A:288:ASN:ND2	2.74	0.41
1:A:213:PRO:N	1:A:214:PRO:CD	2.84	0.41
1:B:269:ILE:N	1:B:269:ILE:CD1	2.84	0.41
1:C:102:ARG:NH2	1:D:169:LYS:O	2.54	0.40
1:F:117:GLU:CG	1:F:118:VAL:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	306/327 (94%)	289 (94%)	17 (6%)	0	100	100
1	B	306/327 (94%)	293 (96%)	12 (4%)	1 (0%)	50	84
1	C	306/327 (94%)	287 (94%)	19 (6%)	0	100	100
1	D	309/327 (94%)	287 (93%)	19 (6%)	3 (1%)	22	58
1	E	306/327 (94%)	276 (90%)	30 (10%)	0	100	100
1	F	306/327 (94%)	279 (91%)	26 (8%)	1 (0%)	50	84
All	All	1839/1962 (94%)	1711 (93%)	123 (7%)	5 (0%)	50	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	PHE
1	D	47	GLN
1	D	323	TYR
1	F	73	ILE
1	B	334	SER

### 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	277/289 (96%)	257 (93%)	20 (7%)	21	48
1	B	277/289 (96%)	262 (95%)	15 (5%)	31	65
1	C	277/289 (96%)	254 (92%)	23 (8%)	16	40
1	D	280/289 (97%)	265 (95%)	15 (5%)	31	65
1	E	277/289 (96%)	260 (94%)	17 (6%)	26	59
1	F	277/289 (96%)	262 (95%)	15 (5%)	31	65
All	All	1665/1734 (96%)	1560 (94%)	105 (6%)	25	57

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	91	SER

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	100	GLU
1	A	149	GLU
1	A	176	LEU
1	A	180	ASN
1	A	186	ASP
1	A	194	PHE
1	A	224	LYS
1	A	244	VAL
1	A	256	LYS
1	A	264	ARG
1	A	269	ILE
1	A	280	LEU
1	A	288	ASN
1	A	317	VAL
1	A	333	VAL
1	A	334	SER
1	A	340	GLU
1	B	58	THR
1	B	90	ASN
1	B	176	LEU
1	B	177	LYS
1	B	194	PHE
1	B	196	PHE
1	B	200	PHE
1	B	224	LYS
1	B	244	VAL
1	B	268	ARG
1	B	269	ILE
1	B	280	LEU
1	B	288	ASN
1	B	340	GLU
1	B	353	GLU
1	C	49	HIS
1	C	58	THR
1	C	90	ASN
1	C	113	VAL
1	C	176	LEU
1	C	180	ASN
1	C	189	ILE
1	C	194	PHE
1	C	196	PHE

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Mol	Chain	Res	Type
1	C	200	PHE
1	C	204	ASN
1	C	244	VAL
1	C	256	LYS
1	C	268	ARG
1	C	269	ILE
1	C	272	TYR
1	C	280	LEU
1	C	283	LYS
1	C	288	ASN
1	C	320	LEU
1	C	339	ARG
1	C	340	GLU
1	C	343	GLN
1	D	46	GLU
1	D	91	SER
1	D	106	VAL
1	D	114	LYS
1	D	176	LEU
1	D	194	PHE
1	D	224	LYS
1	D	242	THR
1	D	269	ILE
1	D	271	PHE
1	D	280	LEU
1	D	288	ASN
1	D	339	ARG
1	D	340	GLU
1	D	353	GLU
1	E	58	THR
1	E	71	ARG
1	E	74	LEU
1	E	90	ASN
1	E	106	VAL
1	E	124	THR
1	E	149	GLU
1	E	176	LEU
1	E	194	PHE
1	E	224	LYS
1	E	231	VAL
1	E	269	ILE
1	E	280	LEU

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Mol	Chain	Res	Type
1	E	290	SER
1	E	317	VAL
1	E	340	GLU
1	E	353	GLU
1	F	71	ARG
1	F	172	VAL
1	F	176	LEU
1	F	180	ASN
1	F	194	PHE
1	F	231	VAL
1	F	242	THR
1	F	256	LYS
1	F	269	ILE
1	F	272	TYR
1	F	280	LEU
1	F	288	ASN
1	F	338	THR
1	F	340	GLU
1	F	353	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	310/327 (94%)	-0.14	3 (0%) 79 81	34, 58, 99, 154	0
1	B	310/327 (94%)	-0.09	7 (2%) 57 60	34, 60, 100, 132	0
1	C	310/327 (94%)	-0.07	4 (1%) 74 76	43, 66, 100, 133	0
1	D	313/327 (95%)	-0.11	3 (0%) 79 81	37, 62, 105, 173	0
1	E	310/327 (94%)	0.21	14 (4%) 32 34	55, 88, 131, 168	0
1	F	310/327 (94%)	0.45	28 (9%) 10 9	46, 100, 149, 182	0
All	All	1863/1962 (94%)	0.04	59 (3%) 45 48	34, 71, 129, 182	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	54	ARG	5.4
1	F	70	ALA	5.4
1	F	68	LYS	4.3
1	D	46	GLU	4.0
1	F	73	ILE	3.7
1	F	271	PHE	3.7
1	E	50	ILE	3.6
1	E	150	LYS	3.5
1	F	310	ASP	3.4
1	E	244	VAL	3.4
1	F	337	TYR	3.3
1	E	196	PHE	3.3
1	F	335	MET	3.2
1	F	326	PRO	3.2
1	F	55	LEU	3.2
1	F	50	ILE	3.1
1	B	339	ARG	3.1
1	F	49	HIS	3.1
1	E	146	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	196	PHE	3.0
1	A	55	LEU	2.9
1	C	339	ARG	2.9
1	F	333	VAL	2.9
1	A	49	HIS	2.9
1	F	339	ARG	2.9
1	F	147	MET	2.8
1	F	150	LYS	2.8
1	F	244	VAL	2.8
1	B	56	LEU	2.7
1	E	140	TYR	2.7
1	E	141	LEU	2.6
1	C	196	PHE	2.6
1	D	202	PHE	2.6
1	F	330	GLU	2.6
1	B	196	PHE	2.5
1	E	243	LEU	2.5
1	F	334	SER	2.5
1	D	323	TYR	2.5
1	E	272	TYR	2.5
1	F	57	LYS	2.4
1	C	343	GLN	2.4
1	F	79	VAL	2.4
1	F	148	LYS	2.4
1	F	53	TYR	2.4
1	C	340	GLU	2.3
1	E	271	PHE	2.3
1	E	74	LEU	2.3
1	F	273	MET	2.3
1	B	71	ARG	2.2
1	E	270	PRO	2.2
1	E	284	PHE	2.2
1	B	74	LEU	2.2
1	F	77	LYS	2.2
1	F	309	GLU	2.1
1	B	54	ARG	2.1
1	B	49	HIS	2.1
1	E	147	MET	2.1
1	A	73	ILE	2.0
1	F	71	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.