



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2021 – 03:03 pm BST

PDB ID : 7AI4  
Title : Crystal structure of the KLC1-TPR domain truncated from its nonTPR region ([A1-B6]-Delta-nonTPR fragment)  
Authors : Menetrey, J.; Llinas, P.  
Deposited on : 2020-09-26  
Resolution : 2.79 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

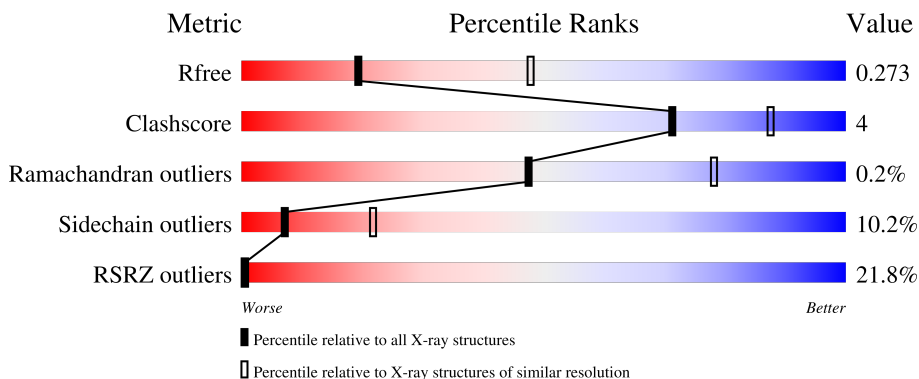
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	293	 14% 70% 12% 17%
1	B	293	 22% 68% 12% 20%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3501 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 Isoform C of Kinesin light chain 1, Isoform C of Kinesin light chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1842	1160	322	355	5	0	0	0
1	B	235	1659	1039	299	316	5	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MET	-	initiating methionine	UNP Q07866
A	176	ARG	-	expression tag	UNP Q07866
A	177	SER	-	expression tag	UNP Q07866
A	178	GLU	-	expression tag	UNP Q07866
A	179	THR	-	expression tag	UNP Q07866
A	180	MET	-	expression tag	UNP Q07866
A	181	SER	-	expression tag	UNP Q07866
A	182	TYR	-	expression tag	UNP Q07866
A	183	TYR	-	expression tag	UNP Q07866
A	184	HIS	-	expression tag	UNP Q07866
A	185	HIS	-	expression tag	UNP Q07866
A	186	HIS	-	expression tag	UNP Q07866
A	187	HIS	-	expression tag	UNP Q07866
A	188	HIS	-	expression tag	UNP Q07866
A	189	HIS	-	expression tag	UNP Q07866
A	190	ASP	-	expression tag	UNP Q07866
A	191	TYR	-	expression tag	UNP Q07866
A	192	ASP	-	expression tag	UNP Q07866
A	193	ILE	-	expression tag	UNP Q07866
A	194	PRO	-	expression tag	UNP Q07866
A	195	THR	-	expression tag	UNP Q07866
A	196	THR	-	expression tag	UNP Q07866
A	197	GLU	-	expression tag	UNP Q07866
A	198	ASN	-	expression tag	UNP Q07866

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Chain	Residue	Modelled	Actual	Comment	Reference
A	199	LEU	-	expression tag	UNP Q07866
A	200	TYR	-	expression tag	UNP Q07866
A	201	PHE	-	expression tag	UNP Q07866
A	202	GLN	-	expression tag	UNP Q07866
A	203	GLY	-	expression tag	UNP Q07866
A	204	ALA	-	expression tag	UNP Q07866
A	205	MET	-	expression tag	UNP Q07866
A	454	GLY	-	linker	UNP Q07866
A	455	GLY	-	linker	UNP Q07866
A	456	GLY	-	linker	UNP Q07866
A	457	GLY	-	linker	UNP Q07866
A	458	SER	-	linker	UNP Q07866
B	175	MET	-	initiating methionine	UNP Q07866
B	176	ARG	-	expression tag	UNP Q07866
B	177	SER	-	expression tag	UNP Q07866
B	178	GLU	-	expression tag	UNP Q07866
B	179	THR	-	expression tag	UNP Q07866
B	180	MET	-	expression tag	UNP Q07866
B	181	SER	-	expression tag	UNP Q07866
B	182	TYR	-	expression tag	UNP Q07866
B	183	TYR	-	expression tag	UNP Q07866
B	184	HIS	-	expression tag	UNP Q07866
B	185	HIS	-	expression tag	UNP Q07866
B	186	HIS	-	expression tag	UNP Q07866
B	187	HIS	-	expression tag	UNP Q07866
B	188	HIS	-	expression tag	UNP Q07866
B	189	HIS	-	expression tag	UNP Q07866
B	190	ASP	-	expression tag	UNP Q07866
B	191	TYR	-	expression tag	UNP Q07866
B	192	ASP	-	expression tag	UNP Q07866
B	193	ILE	-	expression tag	UNP Q07866
B	194	PRO	-	expression tag	UNP Q07866
B	195	THR	-	expression tag	UNP Q07866
B	196	THR	-	expression tag	UNP Q07866
B	197	GLU	-	expression tag	UNP Q07866
B	198	ASN	-	expression tag	UNP Q07866
B	199	LEU	-	expression tag	UNP Q07866
B	200	TYR	-	expression tag	UNP Q07866
B	201	PHE	-	expression tag	UNP Q07866
B	202	GLN	-	expression tag	UNP Q07866
B	203	GLY	-	expression tag	UNP Q07866
B	204	ALA	-	expression tag	UNP Q07866

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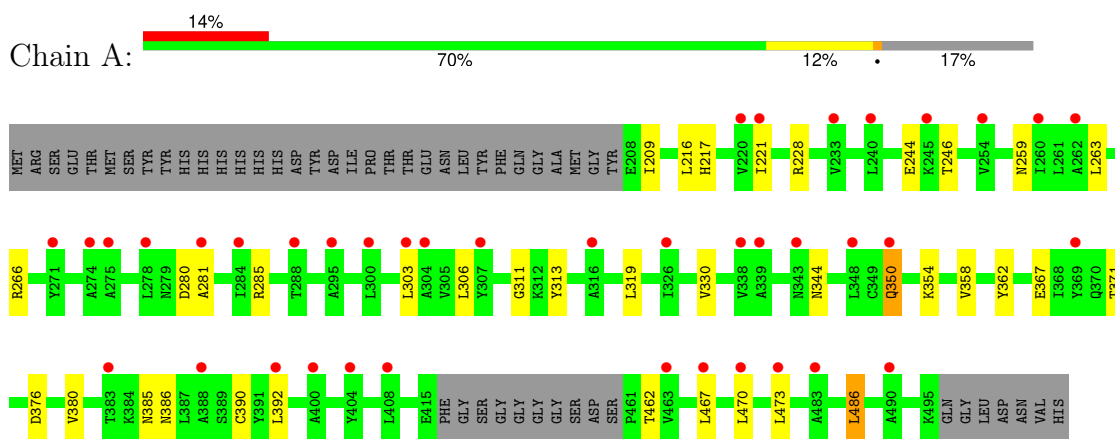
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Chain	Residue	Modelled	Actual	Comment	Reference
B	205	MET	-	expression tag	UNP Q07866
B	454	GLY	-	linker	UNP Q07866
B	455	GLY	-	linker	UNP Q07866
B	456	GLY	-	linker	UNP Q07866
B	457	GLY	-	linker	UNP Q07866
B	458	SER	-	linker	UNP Q07866

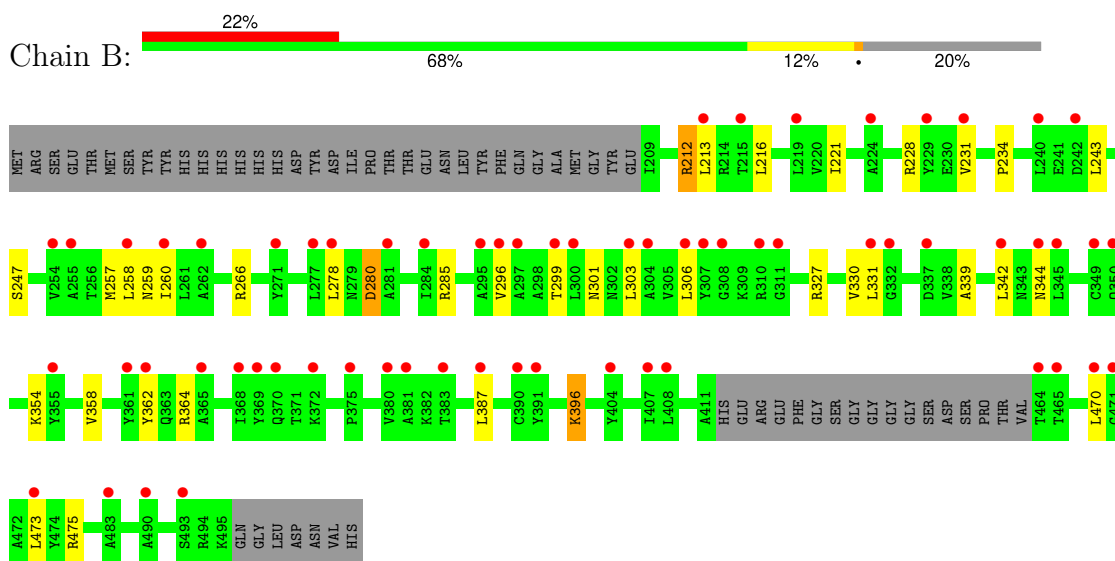
### 3 Residue-property plots [i](#)

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: Isoform C of Kinesin light chain 1, Isoform C of Kinesin light chain 1



- Molecule 1: Isoform C of Kinesin light chain 1, Isoform C of Kinesin light chain 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.22Å 55.82Å 103.57Å 90.00° 108.51° 90.00°	Depositor
Resolution (Å)	49.11 – 2.79 49.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.11-2.79) 99.2 (49.11-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, $R_{free}$	0.217 , 0.252 0.234 , 0.273	Depositor DCC
$R_{free}$ test set	834 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.47	0/1870	0.62	0/2541
1	B	0.40	0/1685	0.54	0/2307
All	All	0.44	0/3555	0.58	0/4848

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	1842	0	1794	10	0
1	B	1659	0	1478	14	0
All	All	3501	0	3272	24	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 4.

All (24) 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:350:GLN:HG3	1:A:358:VAL:HG11	1.69	0.74
1:B:278:LEU:HD12	1:B:306:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:HIS:CE1	1:A:221:ILE:HD12	2.37	0.59
1:B:327:ARG:HA	1:B:330:VAL:HG12	1.85	0.58
1:B:213:LEU:HD21	1:B:243:LEU:HD11	1.86	0.55
1:A:362:TYR:CZ	1:A:386:ASN:HB3	2.43	0.54
1:B:330:VAL:HG13	1:B:331:LEU:HG	1.91	0.52
1:B:212:ARG:NH1	1:B:247:SER:OG	2.43	0.51
1:A:392:LEU:HD13	1:A:473:LEU:HD12	1.91	0.51
1:B:257:MET:HA	1:B:260:ILE:HG22	1.93	0.50
1:A:367:GLU:O	1:A:371:THR:HG23	2.12	0.49
1:B:285:ARG:NH1	1:B:299:THR:OG1	2.43	0.49
1:A:467:LEU:HD23	1:A:486:LEU:HD23	1.96	0.48
1:B:231:VAL:C	1:B:234:PRO:HD2	2.33	0.47
1:B:285:ARG:HB3	1:B:296:VAL:HG22	1.98	0.45
1:B:354:LYS:O	1:B:358:VAL:HG23	2.17	0.44
1:B:362:TYR:HB2	1:B:387:LEU:HD13	2.00	0.44
1:A:470:LEU:HB2	1:A:486:LEU:HD22	2.02	0.42
1:A:303:LEU:HB3	1:A:319:LEU:HD13	2.01	0.42
1:B:258:LEU:HD13	1:B:280:ASP:HB3	2.02	0.41
1:B:339:ALA:HA	1:B:342:LEU:HD12	2.02	0.41
1:B:470:LEU:HD12	1:B:473:LEU:HD23	2.02	0.41
1:A:281:ALA:O	1:A:285:ARG:HG3	2.21	0.41
1:A:311:GLY:HA2	1:A:313:TYR:CZ	2.55	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	239/293 (82%)	234 (98%)	5 (2%)	0	100	100
1	B	231/293 (79%)	217 (94%)	13 (6%)	1 (0%)	34	66
All	All	470/586 (80%)	451 (96%)	18 (4%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	LYS

### 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	A	183/245 (75%)	163 (89%)	20 (11%)	6	19
1	B	140/245 (57%)	127 (91%)	13 (9%)	9	26
All	All	323/490 (66%)	290 (90%)	33 (10%)	7	22

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	ILE
1	A	216	LEU
1	A	228	ARG
1	A	244	GLU
1	A	246	THR
1	A	259	ASN
1	A	263	LEU
1	A	266	ARG
1	A	280	ASP
1	A	306	LEU
1	A	330	VAL
1	A	344	ASN
1	A	350	GLN
1	A	354	LYS
1	A	376	ASP
1	A	380	VAL
1	A	385	ASN
1	A	390	CYS
1	A	462	THR
1	A	486	LEU
1	B	212	ARG
1	B	216	LEU

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Mol	Chain	Res	Type
1	B	221	ILE
1	B	228	ARG
1	B	259	ASN
1	B	266	ARG
1	B	280	ASP
1	B	301	ASN
1	B	303	LEU
1	B	344	ASN
1	B	364	ARG
1	B	396	LYS
1	B	475	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 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

### 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	243/293 (82%)	1.11	40 (16%) <b>1</b> <b>1</b>	71, 97, 124, 132	0
1	B	235/293 (80%)	1.21	64 (27%) <b>0</b> <b>0</b>	100, 125, 159, 175	0
All	All	478/586 (81%)	1.16	104 (21%) <b>0</b> <b>0</b>	71, 112, 148, 175	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	TYR	5.6
1	B	368	ILE	5.1
1	B	483	ALA	4.8
1	B	349	CYS	4.8
1	B	304	ALA	4.3
1	B	229	TYR	3.9
1	B	383	THR	3.9
1	A	388	ALA	3.9
1	B	345	LEU	3.8
1	B	381	ALA	3.6
1	B	404	TYR	3.6
1	B	375	PRO	3.4
1	A	339	ALA	3.3
1	B	362	TYR	3.2
1	B	380	VAL	3.2
1	A	316	ALA	3.2
1	B	224	ALA	3.2
1	B	470	LEU	3.2
1	B	300	LEU	3.1
1	B	407	ILE	3.1
1	B	262	ALA	3.1
1	B	213	LEU	3.1
1	A	300	LEU	3.0
1	B	258	LEU	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	365	ALA	3.0
1	A	490	ALA	2.9
1	B	473	LEU	2.9
1	A	254	VAL	2.9
1	A	271	TYR	2.8
1	B	342	LEU	2.8
1	A	350	GLN	2.8
1	B	390	CYS	2.8
1	B	308	GLY	2.8
1	B	344	ASN	2.7
1	B	295	ALA	2.7
1	B	408	LEU	2.7
1	B	240	LEU	2.7
1	A	307	TYR	2.7
1	B	231	VAL	2.7
1	B	255	ALA	2.7
1	B	471	GLY	2.6
1	A	278	LEU	2.6
1	B	219	LEU	2.6
1	B	311	GLY	2.6
1	A	284	ILE	2.5
1	B	331	LEU	2.5
1	A	220	VAL	2.5
1	B	370	GLN	2.5
1	B	297	ALA	2.5
1	B	391	TYR	2.5
1	A	338	VAL	2.5
1	B	493	SER	2.5
1	A	240	LEU	2.4
1	B	242	ASP	2.4
1	A	473	LEU	2.4
1	B	303	LEU	2.4
1	A	274	ALA	2.4
1	A	463	VAL	2.4
1	B	299	THR	2.3
1	B	337	ASP	2.3
1	A	404	TYR	2.3
1	B	361	TYR	2.3
1	A	369	TYR	2.3
1	B	307	TYR	2.3
1	B	490	ALA	2.3
1	B	372	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	260	ILE	2.3
1	B	465	THR	2.2
1	B	355	TYR	2.2
1	A	233	VAL	2.2
1	B	260	ILE	2.2
1	B	306	LEU	2.2
1	A	221	ILE	2.2
1	A	303	LEU	2.2
1	B	277	LEU	2.2
1	A	245	LYS	2.2
1	B	464	THR	2.2
1	A	326	ILE	2.2
1	B	284	ILE	2.2
1	A	281	ALA	2.2
1	B	310	ARG	2.2
1	A	343	ASN	2.1
1	B	254	VAL	2.1
1	A	304	ALA	2.1
1	A	288	THR	2.1
1	A	408	LEU	2.1
1	B	281	ALA	2.1
1	A	400	ALA	2.1
1	B	350	GLN	2.1
1	A	467	LEU	2.1
1	A	262	ALA	2.1
1	A	483	ALA	2.1
1	B	332	GLY	2.1
1	B	215	THR	2.1
1	B	271	TYR	2.1
1	A	275	ALA	2.0
1	A	470	LEU	2.0
1	B	296	VAL	2.0
1	A	295	ALA	2.0
1	A	383	THR	2.0
1	A	348	LEU	2.0
1	A	392	LEU	2.0
1	B	278	LEU	2.0
1	B	387	LEU	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 [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.