



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:20 PM GMT

PDB ID : 3TPM  
Title : Crystal structure of MAL RPEL domain in complex with importin-alpha  
Authors : Hirano, H.; Matsuura, Y.  
Deposited on : 2011-09-08  
Resolution : 2.10 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.

---

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

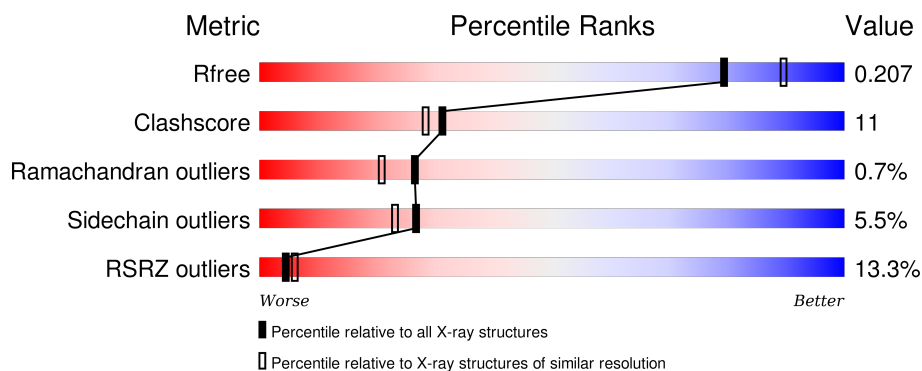
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

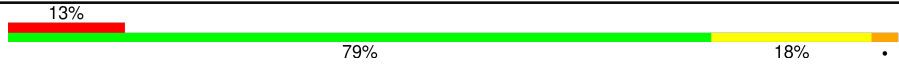

The reported resolution of this entry is 2.10 Å.

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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	422	
2	B	120	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3618 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 Importin subunit alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3220	2052	546	612	10			

- Molecule 2 is a protein called MAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	0	0	0
			119	76	27	16			

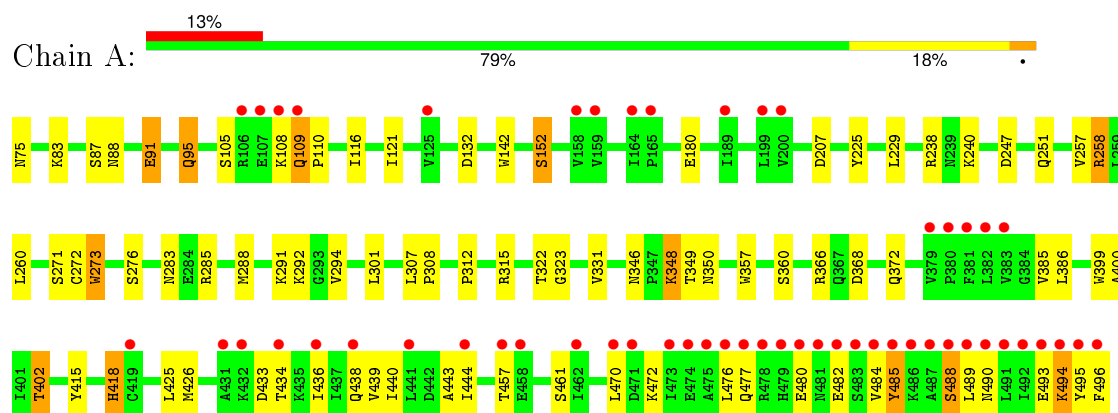
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	265	Total	O	0	0
			265	265		
3	B	14	Total	O	0	0
			14	14		

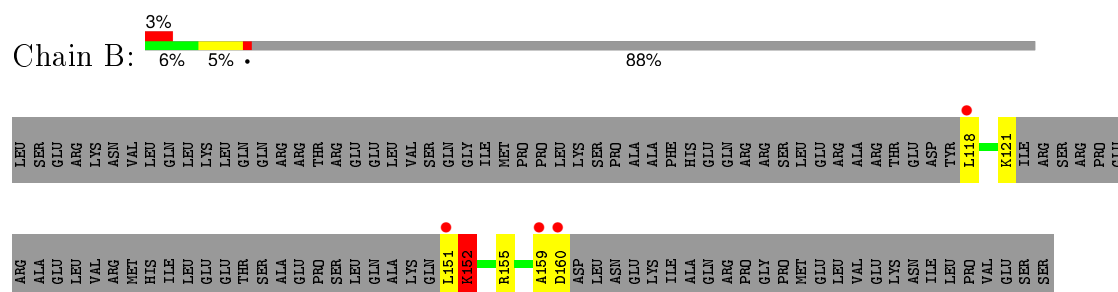
### 3 Residue-property plots [i](#)

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: Importin subunit alpha-2



#### • Molecule 2: MAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.66Å 90.12Å 98.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 2.10 41.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.00-2.10) 98.7 (41.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.166 , 0.208 0.165 , 0.207	Depositor DCC
$R_{free}$ test set	2097 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41136 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	1.11	10/3278 (0.3%)	1.10	9/4467 (0.2%)
2	B	1.01	0/117	1.18	0/149
All	All	1.10	10/3395 (0.3%)	1.11	9/4616 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	TRP	CD2-CE2	6.83	1.49	1.41
1	A	271	SER	CB-OG	-6.59	1.33	1.42
1	A	105	SER	CB-OG	-6.23	1.34	1.42
1	A	258	ARG	CZ-NH1	6.18	1.41	1.33
1	A	357	TRP	CD2-CE2	5.93	1.48	1.41
1	A	418	HIS	CG-CD2	5.57	1.45	1.35
1	A	142	TRP	CD2-CE2	5.47	1.48	1.41
1	A	399	TRP	CD2-CE2	5.37	1.47	1.41
1	A	152	SER	CB-OG	-5.15	1.35	1.42
1	A	415	TYR	CE1-CZ	5.14	1.45	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	A	258	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	A	238	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	240	LYS	C-N-CA	-6.38	105.74	121.70
1	A	87	SER	C-N-CA	-5.46	108.04	121.70
1	A	385	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	A	238	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	271	SER	CB-CA-C	-5.09	100.43	110.10
1	A	260	LEU	CB-CG-CD2	-5.08	102.36	111.00

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	3220	0	3296	64	1
2	B	119	0	147	12	0
3	A	265	0	0	10	1
3	B	14	0	0	2	0
All	All	3618	0	3443	73	1

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 11.

All (73) 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:247:ASP:HB3	3:A:661:HOH:O	1.61	1.00
1:A:477:GLN:HA	1:A:485:TYR:HB2	1.52	0.91
1:A:75:ASN:N	3:A:511:HOH:O	2.05	0.88
1:A:346:ASN:HD22	1:A:348:LYS:H	1.21	0.87
1:A:477:GLN:NE2	1:A:489:LEU:HA	1.92	0.84
2:B:159:ALA:HA	2:B:160:ASP:HB2	1.59	0.81
2:B:151:LEU:O	2:B:151:LEU:HD12	1.80	0.81
1:A:477:GLN:HE21	1:A:489:LEU:HA	1.43	0.80
2:B:152:LYS:HE3	3:B:192:HOH:O	1.83	0.78
2:B:151:LEU:O	2:B:152:LYS:HB3	1.85	0.76
1:A:477:GLN:HE21	1:A:489:LEU:CA	1.99	0.74
1:A:346:ASN:ND2	1:A:348:LYS:H	1.90	0.70
1:A:477:GLN:O	1:A:485:TYR:HD1	1.76	0.69
1:A:434:THR:HG21	3:A:576:HOH:O	1.92	0.69
1:A:493:GLU:O	1:A:495:TYR:N	2.28	0.67
1:A:386:LEU:HD21	1:A:425:LEU:HD13	1.77	0.65
1:A:472:LYS:O	1:A:476:LEU:HG	1.96	0.65
1:A:470:LEU:HD13	1:A:496:PHE:CD1	2.33	0.63
1:A:272:CYS:HB3	1:A:312:PRO:HB2	1.81	0.63
1:A:477:GLN:O	1:A:485:TYR:CD1	2.52	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HB3	1:A:308:PRO:HD3	1.82	0.62
1:A:348:LYS:HE3	1:A:350:ASN:HB3	1.82	0.60
1:A:292:LYS:NZ	3:A:653:HOH:O	2.33	0.60
1:A:75:ASN:N	3:A:525:HOH:O	2.35	0.59
1:A:426:MET:HE1	1:A:444:ILE:HD12	1.82	0.59
1:A:477:GLN:HA	1:A:485:TYR:CB	2.28	0.59
1:A:426:MET:CE	1:A:444:ILE:HD12	2.32	0.59
1:A:402:THR:HB	1:A:443:ALA:HB2	1.84	0.59
1:A:132:ASP:HB2	3:A:54:HOH:O	2.03	0.57
1:A:402:THR:HG21	1:A:439:VAL:O	2.05	0.56
1:A:285:ARG:HA	1:A:288:MET:HE3	1.87	0.56
2:B:151:LEU:CD1	2:B:151:LEU:O	2.54	0.54
1:A:485:TYR:HA	1:A:488:SER:OG	2.07	0.54
1:A:276:SER:HB2	1:A:315:ARG:HG3	1.91	0.52
1:A:322:THR:HB	2:B:121:LYS:HG2	1.91	0.52
1:A:426:MET:HE2	1:A:444:ILE:CD1	2.39	0.52
1:A:457:THR:O	1:A:461:SER:HB2	2.12	0.49
1:A:292:LYS:HE2	3:A:21:HOH:O	2.11	0.49
1:A:440:ILE:O	1:A:444:ILE:HG12	2.12	0.48
1:A:418:HIS:HB2	3:A:48:HOH:O	2.12	0.48
1:A:348:LYS:HE3	1:A:350:ASN:H	1.79	0.47
1:A:285:ARG:HD2	3:A:52:HOH:O	2.14	0.47
1:A:426:MET:HE2	1:A:444:ILE:HD11	1.96	0.47
1:A:426:MET:CE	1:A:444:ILE:CD1	2.91	0.47
1:A:402:THR:CG2	1:A:439:VAL:CG1	2.93	0.47
1:A:368:ASP:O	1:A:372:GLN:HG3	2.15	0.47
1:A:109:GLN:HA	1:A:110:PRO:HD2	1.67	0.46
1:A:350:ASN:HB2	3:A:683:HOH:O	2.15	0.46
1:A:257:VAL:HG22	1:A:294:VAL:CG1	2.46	0.45
1:A:285:ARG:HD3	1:A:288:MET:CE	2.46	0.45
2:B:159:ALA:CA	2:B:160:ASP:HB2	2.40	0.44
1:A:91:GLU:O	1:A:95:GLN:HG2	2.16	0.44
1:A:307:LEU:N	1:A:308:PRO:CD	2.81	0.44
2:B:151:LEU:O	2:B:152:LYS:CB	2.55	0.44
1:A:490:ASN:O	1:A:494:LYS:HB2	2.17	0.43
1:A:283:ASN:OD1	1:A:323:GLY:HA2	2.18	0.43
1:A:273:TRP:CD1	2:B:151:LEU:HD22	2.53	0.43
1:A:402:THR:HG21	1:A:439:VAL:CG1	2.50	0.42
1:A:207:ASP:OD1	1:A:251:GLN:NE2	2.52	0.42
1:A:402:THR:CG2	1:A:439:VAL:HG13	2.50	0.42
1:A:366:ARG:HD2	1:A:368:ASP:OD1	2.20	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:TYR:CE2	1:A:229:LEU:HD11	2.55	0.42
1:A:322:THR:HG21	2:B:121:LYS:HA	2.01	0.42
1:A:476:LEU:O	1:A:485:TYR:HB3	2.19	0.41
1:A:433:ASP:HB3	1:A:436:ILE:HG22	2.01	0.41
1:A:360:SER:HA	1:A:400:ALA:HA	2.02	0.41
1:A:402:THR:CG2	1:A:439:VAL:HG12	2.51	0.41
1:A:180:GLU:HB2	1:A:225:TYR:CD1	2.55	0.41
1:A:301:LEU:HA	1:A:301:LEU:HD23	1.86	0.41
1:A:477:GLN:HG3	1:A:488:SER:HB2	2.02	0.41
2:B:152:LYS:HG2	2:B:155:ARG:HG3	2.03	0.41
2:B:152:LYS:CE	3:B:192:HOH:O	2.57	0.40
1:A:116:ILE:HG12	1:A:121:ILE:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:OE1	3:A:679:HOH:O[3_554]	2.00	0.20

## 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	420/422 (100%)	400 (95%)	18 (4%)	2 (0%)	34	30
2	B	10/120 (8%)	9 (90%)	0	1 (10%)	1	0
All	All	430/542 (79%)	409 (95%)	18 (4%)	3 (1%)	26	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	LYS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	484	VAL
2	B	152	LYS

### 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	354/354 (100%)	336 (95%)	18 (5%)	29	26
2	B	12/109 (11%)	10 (83%)	2 (17%)	3	1
All	All	366/463 (79%)	346 (94%)	20 (6%)	27	23

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

Mol	Chain	Res	Type
1	A	83	LYS
1	A	88	ASN
1	A	91	GLU
1	A	95	GLN
1	A	108	LYS
1	A	109	GLN
1	A	152	SER
1	A	258	ARG
1	A	291	LYS
1	A	331	VAL
1	A	348	LYS
1	A	349	THR
1	A	402	THR
1	A	438	GLN
1	A	480	GLU
1	A	482	GLU
1	A	485	TYR
1	A	488	SER
2	B	118	LEU
2	B	152	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	95	GLN
1	A	261	HIS
1	A	346	ASN
1	A	438	GLN
1	A	477	GLN
1	A	479	HIS

### 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	422/422 (100%)	0.69	54 (12%) 5 6	26, 40, 91, 117	0
2	B	14/120 (11%)	1.24	4 (28%) 1 1	36, 73, 88, 88	0
All	All	436/542 (80%)	0.71	58 (13%) 4 6	26, 40, 91, 117	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	10.0
1	A	496	PHE	8.4
1	A	476	LEU	7.1
1	A	489	LEU	6.9
1	A	484	VAL	6.6
1	A	491	LEU	6.5
1	A	492	ILE	6.5
1	A	478	ARG	5.8
1	A	479	HIS	5.3
1	A	495	TYR	5.2
1	A	477	GLN	5.0
1	A	475	ALA	5.0
1	A	107	GLU	4.9
1	A	473	ILE	4.9
1	A	480	GLU	4.8
1	A	482	GLU	4.7
1	A	432	LYS	4.6
1	A	486	LYS	4.5
1	A	493	GLU	4.3
1	A	474	GLU	4.1
2	B	160	ASP	4.1
1	A	490	ASN	4.1
1	A	487	ALA	4.0
1	A	108	LYS	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	483	SER	3.8
1	A	436	ILE	3.8
1	A	470	LEU	3.7
1	A	434	THR	3.5
1	A	441	LEU	3.4
2	B	159	ALA	3.3
1	A	109	GLN	3.3
1	A	494	LYS	3.2
1	A	431	ALA	3.0
1	A	488	SER	3.0
1	A	158	VAL	3.0
1	A	380	PRO	3.0
2	B	151	LEU	2.9
1	A	159	VAL	2.9
1	A	379	VAL	2.9
1	A	199	LEU	2.8
1	A	481	ASN	2.6
1	A	457	THR	2.6
1	A	438	GLN	2.6
1	A	189	ILE	2.5
1	A	471	ASP	2.4
1	A	444	ILE	2.4
1	A	419	CYS	2.4
1	A	106	ARG	2.4
1	A	200	VAL	2.4
1	A	462	ILE	2.3
1	A	165	PRO	2.2
1	A	381	PHE	2.1
2	B	118	LEU	2.1
1	A	382	LEU	2.1
1	A	164	ILE	2.1
1	A	458	GLU	2.0
1	A	125	VAL	2.0
1	A	383	VAL	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 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.