



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:01 pm GMT

PDB ID : 4L6U  
Title : Crystal structure of AF1868: Cmr1 subunit of the Cmr RNA silencing complex  
Authors : Sun, J.; Jeon, J.H.; Shin, M.; Shin, H.C.; Oh, B.H.; Kim, J.S.  
Deposited on : 2013-06-12  
Resolution : 2.50 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

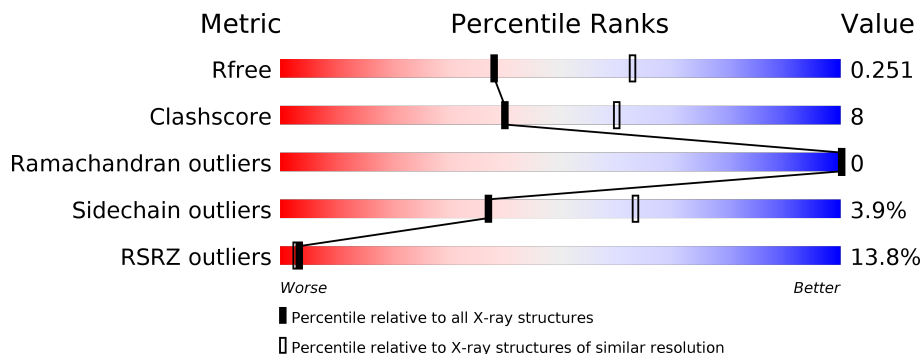
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	329	<div> <div>13%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	B	329	<div> <div>12%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>• 12%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4638 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2369	1533	397	428	11			
1	B	288	Total	C	N	O	S	0	0	0
			2264	1464	374	414	12			

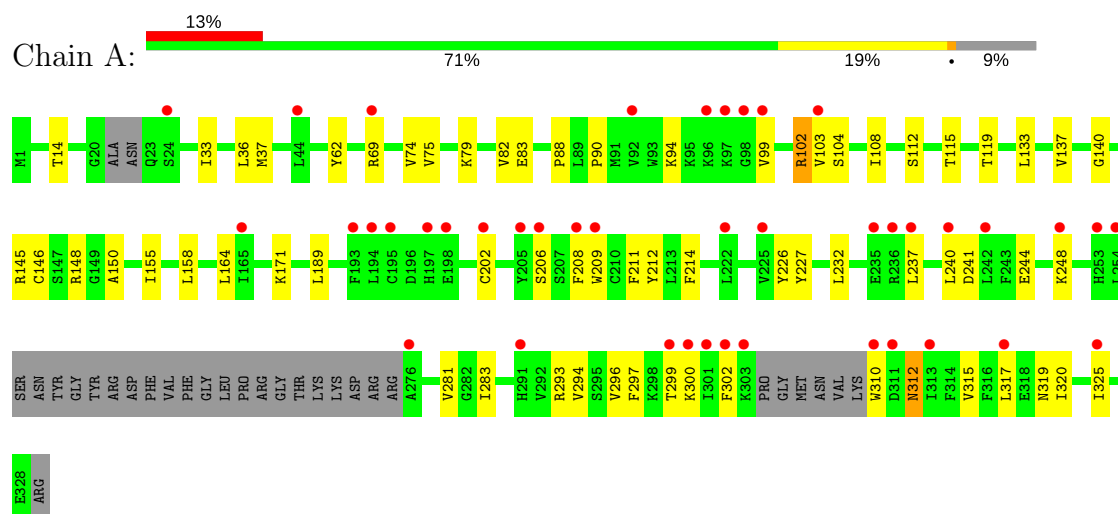
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	1	Total	O	0	0
			1	1		

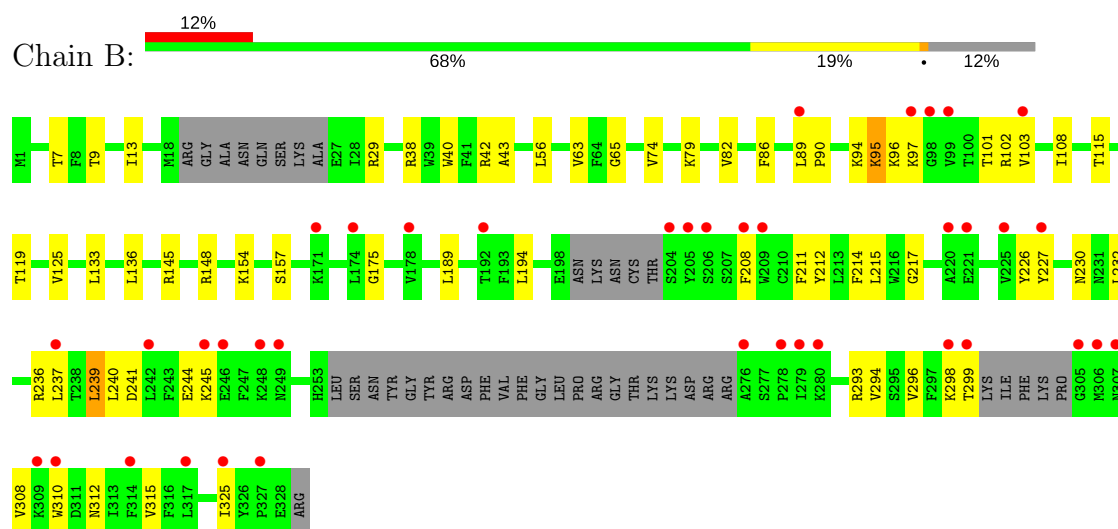
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Putative uncharacterized protein



#### • Molecule 1: Putative uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.69Å 64.16Å 79.28Å 90.00° 93.79° 90.00°	Depositor
Resolution (Å)	79.10 – 2.50 79.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (79.10-2.50) 81.4 (79.10-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.230 , 0.253 0.231 , 0.251	Depositor DCC
$R_{free}$ test set	2429 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 77.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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	0.23	0/2416	0.38	0/3253
1	B	0.24	0/2308	0.42	0/3114
All	All	0.23	0/4724	0.40	0/6367

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	2369	0	2348	37	0
1	B	2264	0	2224	39	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
All	All	4638	0	4572	76	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 8.

All (76) 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:B:95:LYS:HB2	1:B:96:LYS:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:O	1:B:245:LYS:NZ	2.18	0.76
1:A:208:PHE:HA	1:A:211:PHE:HB2	1.67	0.75
1:A:226:TYR:HA	1:A:240:LEU:HD12	1.70	0.72
1:B:102:ARG:NH2	1:B:244:GLU:OE2	2.25	0.69
1:B:217:GLY:HA3	1:B:239:LEU:HD11	1.79	0.65
1:B:94:LYS:HB2	1:B:103:VAL:HG12	1.80	0.64
1:B:208:PHE:HA	1:B:211:PHE:HB2	1.79	0.64
1:A:140:GLY:O	1:A:293:ARG:NH2	2.31	0.61
1:A:82:VAL:HG13	1:A:108:ILE:HG23	1.84	0.59
1:A:79:LYS:HB2	1:A:115:THR:HB	1.84	0.59
1:A:90:PRO:HG2	1:A:145:ARG:HB3	1.84	0.58
1:B:102:ARG:NH1	1:B:241:ASP:OD1	2.36	0.58
1:B:145:ARG:HH12	1:B:148:ARG:HH11	1.50	0.57
1:A:299:THR:OG1	1:A:300:LYS:N	2.39	0.56
1:B:232:LEU:HB3	1:B:245:LYS:HE2	1.88	0.54
1:B:95:LYS:CB	1:B:96:LYS:HA	2.35	0.53
1:A:281:VAL:HG12	1:A:294:VAL:HG22	1.90	0.52
1:A:232:LEU:HA	1:A:237:LEU:HD21	1.91	0.52
1:A:214:PHE:HB2	1:A:294:VAL:HB	1.91	0.52
1:B:82:VAL:HG13	1:B:108:ILE:HG23	1.89	0.52
1:B:90:PRO:HG2	1:B:145:ARG:HB3	1.90	0.52
1:B:38:ARG:NH2	1:B:65:GLY:O	2.38	0.52
1:A:299:THR:HG21	1:A:302:PHE:HB2	1.93	0.51
1:A:312:ASN:HA	1:A:315:VAL:HG22	1.93	0.50
1:B:226:TYR:HA	1:B:240:LEU:HD12	1.93	0.50
1:B:312:ASN:HA	1:B:315:VAL:HG22	1.93	0.50
1:A:94:LYS:HG3	1:A:103:VAL:HG22	1.94	0.50
1:B:212:TYR:HB2	1:B:296:VAL:HB	1.94	0.49
1:A:240:LEU:HD11	1:A:283:ILE:HD11	1.94	0.49
1:A:88:PRO:HA	1:A:104:SER:HA	1.95	0.49
1:A:202:CYS:HA	1:A:209:TRP:NE1	2.27	0.49
1:B:237:LEU:HD22	1:B:245:LYS:HE3	1.95	0.48
1:A:62:TYR:HD1	1:A:69:ARG:HH22	1.61	0.48
1:B:63:VAL:HG13	1:B:125:VAL:HG13	1.95	0.48
1:A:212:TYR:HB2	1:A:296:VAL:HB	1.96	0.48
1:A:14:THR:HG21	1:A:283:ILE:HD13	1.95	0.48
1:B:227:TYR:CE2	1:B:240:LEU:HB3	2.49	0.48
1:A:237:LEU:HD22	1:A:241:ASP:HB3	1.96	0.47
1:B:96:LYS:HA	1:B:97:LYS:HA	1.53	0.47
1:B:95:LYS:HB2	1:B:97:LYS:HA	1.97	0.47
1:A:74:VAL:HB	1:A:119:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PHE:HB2	1:B:294:VAL:HB	1.97	0.46
1:A:90:PRO:HG3	1:A:150:ALA:HB2	1.98	0.45
1:A:148:ARG:HA	1:A:148:ARG:HD3	1.77	0.45
1:B:237:LEU:CD2	1:B:245:LYS:HE3	2.46	0.45
1:B:175:GLY:HA3	1:B:325:ILE:HG22	1.97	0.45
1:A:227:TYR:CE2	1:A:240:LEU:HD13	2.52	0.45
1:B:89:LEU:HD13	1:B:103:VAL:HG23	1.99	0.45
1:B:215:LEU:HD23	1:B:293:ARG:HA	1.99	0.45
1:A:33:ILE:HG22	1:A:37:MET:HE2	1.99	0.45
1:B:230:ASN:N	1:B:230:ASN:OD1	2.49	0.44
1:B:13:ILE:HD11	1:B:154:LYS:HB3	1.99	0.44
1:B:298:LYS:HA	1:B:310:TRP:NE1	2.32	0.44
1:B:194:LEU:HD23	1:B:194:LEU:H	1.82	0.44
1:A:82:VAL:HA	1:A:112:SER:HB3	2.00	0.43
1:B:43:ALA:O	1:B:208:PHE:N	2.50	0.43
1:A:158:LEU:HD21	1:A:164:LEU:HD12	2.01	0.43
1:A:244:GLU:HG2	1:A:248:LYS:HE3	2.00	0.43
1:A:102:ARG:NH1	1:A:227:TYR:HB3	2.34	0.42
1:B:79:LYS:HB2	1:B:115:THR:HB	2.01	0.42
1:B:40:TRP:CD1	1:B:136:LEU:HD23	2.54	0.42
1:B:42:ARG:HA	1:B:56:LEU:HD11	2.00	0.42
1:A:202:CYS:HA	1:A:209:TRP:HE1	1.84	0.42
1:B:74:VAL:HB	1:B:119:THR:HG23	2.01	0.42
1:A:37:MET:HE3	1:A:75:VAL:HG21	2.01	0.42
1:A:317:LEU:HD23	1:A:320:ILE:HD11	2.02	0.41
1:A:312:ASN:N	1:A:312:ASN:OD1	2.39	0.41
1:B:101:THR:HG22	1:B:230:ASN:HD22	1.85	0.41
1:A:102:ARG:NH2	1:A:244:GLU:OE2	2.54	0.41
1:B:227:TYR:CZ	1:B:240:LEU:HB3	2.55	0.41
1:A:137:VAL:HG11	1:A:155:ILE:HG13	2.03	0.41
1:A:171:LYS:HB3	1:A:325:ILE:HD13	2.02	0.41
1:B:9:THR:HB	1:B:157:SER:HB2	2.03	0.41
1:B:299:THR:O	1:B:299:THR:OG1	2.31	0.41
1:A:206:SER:HA	1:A:297:PHE:HB3	2.03	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	289/329 (88%)	277 (96%)	12 (4%)	0	100	100
1	B	278/329 (84%)	265 (95%)	13 (5%)	0	100	100
All	All	567/658 (86%)	542 (96%)	25 (4%)	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	251/292 (86%)	241 (96%)	10 (4%)	36	62
1	B	239/292 (82%)	230 (96%)	9 (4%)	38	64
All	All	490/584 (84%)	471 (96%)	19 (4%)	37	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	83	GLU
1	A	99	VAL
1	A	102	ARG
1	A	133	LEU
1	A	146	CYS
1	A	189	LEU
1	A	310	TRP

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Mol	Chain	Res	Type
1	A	312	ASN
1	A	319	ASN
1	B	7	THR
1	B	29	ARG
1	B	86	PHE
1	B	95	LYS
1	B	133	LEU
1	B	189	LEU
1	B	236	ARG
1	B	239	LEU
1	B	308	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	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 ⓘ

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	299/329 (90%)	0.97	42 (14%) 3 3	59, 99, 180, 235	0
1	B	288/329 (87%)	0.94	39 (13%) 3 3	57, 100, 182, 230	0
All	All	587/658 (89%)	0.96	81 (13%) 3 3	57, 99, 182, 235	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	13.4
1	B	204	SER	12.2
1	A	301	ILE	10.1
1	B	305	GLY	9.4
1	A	205	TYR	8.9
1	A	194	LEU	8.7
1	B	306	MET	7.9
1	A	195	CYS	7.7
1	B	276	ALA	6.7
1	A	302	PHE	6.5
1	B	310	TRP	6.2
1	A	208	PHE	6.2
1	B	307	ASN	6.1
1	A	96	LYS	5.9
1	B	97	LYS	5.7
1	A	97	LYS	5.2
1	B	205	TYR	5.2
1	B	248	LYS	5.1
1	A	310	TRP	5.0
1	B	208	PHE	4.9
1	B	209	TRP	4.5
1	A	276	ALA	4.2
1	B	299	THR	4.2
1	A	92	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	235	GLU	4.1
1	A	325	ILE	3.9
1	A	209	TRP	3.9
1	B	298	LYS	3.9
1	A	69	ARG	3.9
1	A	253	HIS	3.8
1	B	249	ASN	3.7
1	A	291	HIS	3.6
1	A	236	ARG	3.5
1	A	202	CYS	3.5
1	A	206	SER	3.5
1	B	192	THR	3.4
1	B	278	PRO	3.4
1	A	299	THR	3.3
1	A	300	LYS	3.2
1	B	171	LYS	3.2
1	A	24	SER	3.2
1	A	99	VAL	3.2
1	A	240	LEU	3.2
1	A	317	LEU	3.1
1	B	309	LYS	3.1
1	B	325	ILE	3.1
1	B	174	LEU	3.1
1	A	193	PHE	3.1
1	B	242	LEU	3.0
1	B	245	LYS	3.0
1	B	314	PHE	3.0
1	B	227	TYR	2.9
1	A	103	VAL	2.9
1	B	327	PRO	2.8
1	B	317	LEU	2.8
1	A	197	HIS	2.8
1	A	44	LEU	2.6
1	A	165	ILE	2.6
1	A	198	GLU	2.5
1	B	220	ALA	2.5
1	A	225	VAL	2.5
1	B	237	LEU	2.5
1	B	98	GLY	2.5
1	A	222	LEU	2.4
1	B	89	LEU	2.4
1	A	248	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	279	ILE	2.3
1	A	313	ILE	2.3
1	B	178	VAL	2.3
1	A	303	LYS	2.3
1	B	103	VAL	2.3
1	A	237	LEU	2.3
1	B	99	VAL	2.2
1	A	242	LEU	2.2
1	B	280	LYS	2.2
1	B	206	SER	2.2
1	B	221	GLU	2.1
1	A	254	LEU	2.1
1	B	246	GLU	2.1
1	A	311	ASP	2.1
1	B	225	VAL	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.