



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID : 3U8Z  
Title : human merlin FERM domain  
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Deposited on : 2011-10-17  
Resolution : 2.64 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

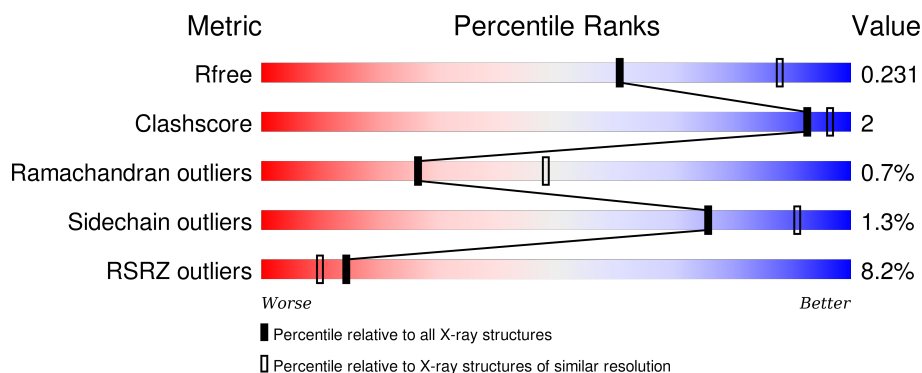
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	300	<div> <div>4%</div> <div>80%7%13%</div> </div>
1	B	300	<div> <div>9%</div> <div>80%6%13%</div> </div>
1	C	300	<div> <div>4%</div> <div>82%6%11%</div> </div>
1	D	300	<div> <div>12%</div> <div>74%5%21%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9077 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 Merlin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2173	1411	362	387	13			
1	B	260	Total	C	N	O	S	0	0	0
			2172	1411	361	387	13			
1	C	266	Total	C	N	O	S	0	0	0
			2222	1443	369	397	13			
1	D	237	Total	C	N	O	S	0	0	0
			1973	1288	324	350	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	EXPRESSION TAG	UNP P35240
A	14	PRO	-	EXPRESSION TAG	UNP P35240
A	15	LEU	-	EXPRESSION TAG	UNP P35240
A	16	GLY	-	EXPRESSION TAG	UNP P35240
A	17	SER	-	EXPRESSION TAG	UNP P35240
B	13	GLY	-	EXPRESSION TAG	UNP P35240
B	14	PRO	-	EXPRESSION TAG	UNP P35240
B	15	LEU	-	EXPRESSION TAG	UNP P35240
B	16	GLY	-	EXPRESSION TAG	UNP P35240
B	17	SER	-	EXPRESSION TAG	UNP P35240
C	13	GLY	-	EXPRESSION TAG	UNP P35240
C	14	PRO	-	EXPRESSION TAG	UNP P35240
C	15	LEU	-	EXPRESSION TAG	UNP P35240
C	16	GLY	-	EXPRESSION TAG	UNP P35240
C	17	SER	-	EXPRESSION TAG	UNP P35240
D	13	GLY	-	EXPRESSION TAG	UNP P35240
D	14	PRO	-	EXPRESSION TAG	UNP P35240
D	15	LEU	-	EXPRESSION TAG	UNP P35240
D	16	GLY	-	EXPRESSION TAG	UNP P35240
D	17	SER	-	EXPRESSION TAG	UNP P35240

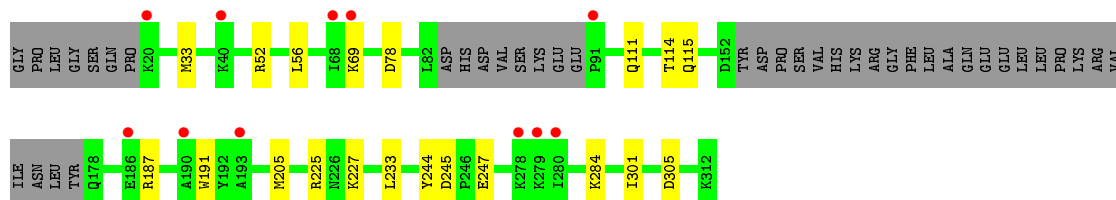
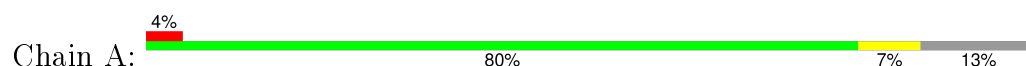
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	164	Total 164	O 164	0	0
2	B	141	Total 141	O 141	0	0
2	C	162	Total 162	O 162	0	0
2	D	70	Total 70	O 70	0	0

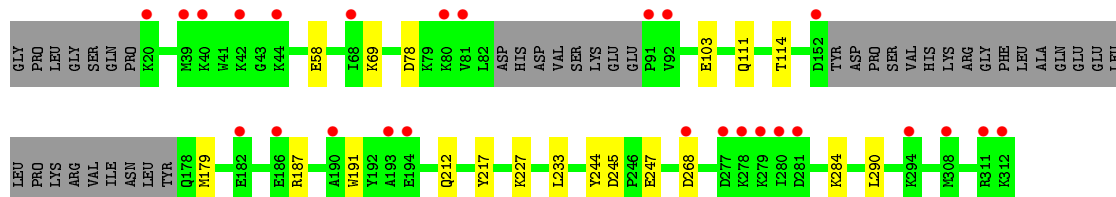
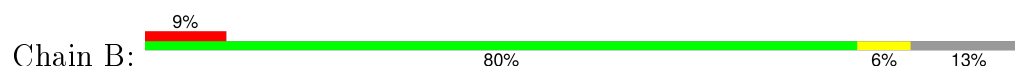
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

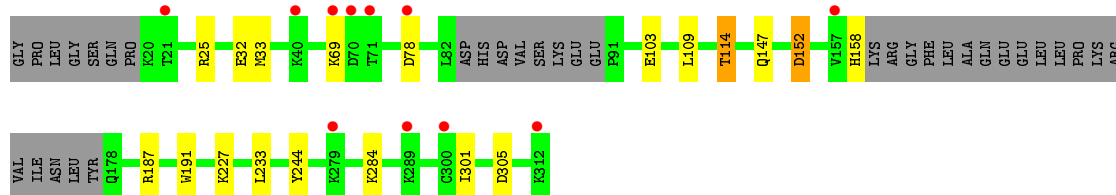
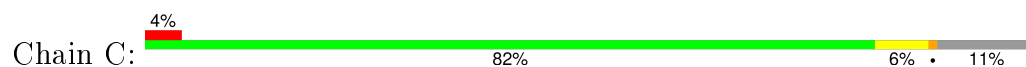
#### • Molecule 1: Merlin



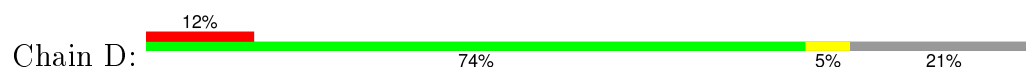
#### • Molecule 1: Merlin

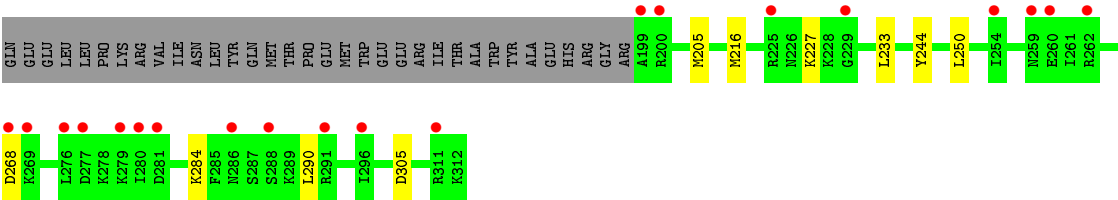


#### • Molecule 1: Merlin



#### • Molecule 1: Merlin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.45Å 105.45Å 330.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.36 – 2.64 26.28 – 2.64	Depositor EDS
% Data completeness (in resolution range)	94.1 (26.36-2.64) 94.2 (26.28-2.64)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.64Å)	Xtriage
Refinement program	BUSTER 2.13.0	Depositor
R, $R_{free}$	0.200 , 0.229 0.204 , 0.231	Depositor DCC
$R_{free}$ test set	2666 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 75.9	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 52476 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.44 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.1713e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.43	0/2223	0.54	0/2992
1	B	0.41	0/2222	0.53	0/2990
1	C	0.43	0/2275	0.56	0/3064
1	D	0.40	0/2016	0.54	0/2711
All	All	0.42	0/8736	0.54	0/11757

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	2173	0	2185	16	0
1	B	2172	0	2184	9	0
1	C	2222	0	2225	11	0
1	D	1973	0	2007	7	0
2	A	164	0	0	2	0
2	B	141	0	0	1	0
2	C	162	0	0	0	0
2	D	70	0	0	0	0
All	All	9077	0	8601	34	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 (34) 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:56:LEU:CD1	1:A:114:THR:HG22	2.02	0.90
1:A:52:ARG:HD3	1:C:152:ASP:OD2	1.81	0.80
1:B:58:GLU:OE1	1:B:114:THR:HG21	1.89	0.72
1:C:25:ARG:HE	1:C:32:GLU:HG3	1.57	0.69
1:A:56:LEU:HD12	1:A:114:THR:HG22	1.74	0.67
1:D:227:LYS:HE3	1:D:284:LYS:H	1.61	0.66
1:A:227:LYS:HE3	1:A:284:LYS:HD3	1.85	0.58
1:B:227:LYS:HE3	1:B:284:LYS:HD3	1.87	0.56
1:D:25:ARG:HH11	1:D:32:GLU:CD	2.09	0.55
1:B:233:LEU:HB2	1:B:244:TYR:HB2	1.90	0.54
1:C:227:LYS:HE3	1:C:284:LYS:HD3	1.89	0.53
1:A:233:LEU:HB2	1:A:244:TYR:HB2	1.91	0.52
1:C:233:LEU:HB2	1:C:244:TYR:HB2	1.92	0.52
1:D:115:GLN:HG3	1:D:205:MET:HE2	1.92	0.52
1:D:233:LEU:HB2	1:D:244:TYR:HB2	1.92	0.51
1:A:301:ILE:HD11	1:C:187:ARG:HE	1.76	0.50
1:A:247:GLU:O	1:B:247:GLU:O	2.30	0.50
1:A:111:GLN:HB2	1:A:114:THR:HG23	1.94	0.49
1:B:191:TRP:HB3	1:D:305:ASP:OD2	2.12	0.49
1:A:187:ARG:HE	1:C:301:ILE:HD11	1.78	0.49
1:D:227:LYS:H	1:D:227:LYS:HD2	1.78	0.48
1:B:111:GLN:O	1:B:114:THR:HG22	2.13	0.47
1:A:191:TRP:HB3	1:C:305:ASP:OD2	2.15	0.47
1:B:179:MET:HE2	1:B:187:ARG:NE	2.30	0.46
1:B:245:ASP:HB3	2:B:357:HOH:O	2.16	0.45
1:A:245:ASP:HB3	2:A:362:HOH:O	2.18	0.43
1:A:305:ASP:OD2	1:C:191:TRP:HB3	2.19	0.43
1:A:115:GLN:HG3	1:A:205:MET:HE2	2.01	0.43
1:B:212:GLN:HA	1:B:217:TYR:CD1	2.56	0.41
1:D:216:MET:HG3	1:D:250:LEU:HD23	2.02	0.41
1:A:187:ARG:HE	1:C:301:ILE:CD1	2.33	0.41
1:A:33:MET:HG2	1:C:33:MET:HB3	2.02	0.41
1:C:109:LEU:HD22	1:C:114:THR:HG22	2.02	0.41
1:A:225:ARG:HD3	2:A:343:HOH:O	2.21	0.40

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	254/300 (85%)	249 (98%)	4 (2%)	1 (0%)	39	63
1	B	254/300 (85%)	249 (98%)	3 (1%)	2 (1%)	24	44
1	C	260/300 (87%)	250 (96%)	8 (3%)	2 (1%)	24	44
1	D	231/300 (77%)	228 (99%)	1 (0%)	2 (1%)	21	40
All	All	999/1200 (83%)	976 (98%)	16 (2%)	7 (1%)	26	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	ASP
1	D	69	LYS
1	A	69	LYS
1	B	69	LYS
1	C	69	LYS
1	B	268	ASP
1	D	268	ASP

### 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	235/271 (87%)	234 (100%)	1 (0%)	93	98
1	B	234/271 (86%)	231 (99%)	3 (1%)	76	91
1	C	240/271 (89%)	235 (98%)	5 (2%)	61	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	215/271 (79%)	212 (99%)	3 (1%)	74	90
All	All	924/1084 (85%)	912 (99%)	12 (1%)	76	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	B	78	ASP
1	B	103	GLU
1	B	290	LEU
1	C	78	ASP
1	C	103	GLU
1	C	114	THR
1	C	147	GLN
1	C	158	HIS
1	D	78	ASP
1	D	114	THR
1	D	290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	147	GLN
1	A	195	HIS
1	B	115	GLN
1	B	147	GLN
1	B	195	HIS
1	C	115	GLN
1	C	147	GLN
1	C	195	HIS
1	D	115	GLN
1	D	147	GLN

### 5.3.3 RNA ⓘ

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	260/300 (86%)	-0.11	11 (4%) 40 33	28, 43, 85, 110	0
1	B	260/300 (86%)	0.26	26 (10%) 9 6	28, 61, 125, 156	0
1	C	266/300 (88%)	-0.03	11 (4%) 41 34	29, 51, 97, 122	0
1	D	237/300 (79%)	0.62	36 (15%) 3 1	48, 80, 138, 169	0
All	All	1023/1200 (85%)	0.17	84 (8%) 14 10	28, 58, 122, 169	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	ILE	7.8
1	C	279	LYS	5.5
1	D	70	ASP	5.3
1	B	279	LYS	4.9
1	D	150	TYR	4.9
1	B	312	LYS	4.6
1	D	22	PHE	4.5
1	C	78	ASP	4.3
1	B	190	ALA	4.2
1	C	70	ASP	4.1
1	B	40	LYS	4.1
1	D	40	LYS	4.1
1	B	193	ALA	4.0
1	A	278	LYS	3.8
1	D	288	SER	3.7
1	A	68	ILE	3.7
1	D	291	ARG	3.7
1	C	289	LYS	3.4
1	A	279	LYS	3.4
1	D	146	VAL	3.4
1	D	21	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	3.3
1	B	39	MET	3.3
1	D	262	ARG	3.3
1	D	268	ASP	3.2
1	D	200	ARG	3.2
1	D	68	ILE	3.2
1	B	277	ASP	3.2
1	D	277	ASP	3.2
1	B	44	LYS	3.2
1	D	20	LYS	3.1
1	D	78	ASP	3.1
1	D	280	ILE	3.1
1	D	254	ILE	3.0
1	D	229	GLY	3.0
1	D	260	GLU	2.9
1	D	80	LYS	2.9
1	D	286	ASN	2.9
1	B	152	ASP	2.9
1	A	69	LYS	2.9
1	A	280	ILE	2.9
1	B	91	PRO	2.8
1	B	92	VAL	2.7
1	D	79	LYS	2.7
1	D	281	ASP	2.7
1	D	39	MET	2.6
1	C	71	THR	2.6
1	D	199	ALA	2.6
1	B	186	GLU	2.6
1	B	80	LYS	2.5
1	C	40	LYS	2.5
1	D	69	LYS	2.5
1	B	42	LYS	2.5
1	B	182	GLU	2.5
1	B	268	ASP	2.4
1	B	81	VAL	2.4
1	B	281	ASP	2.4
1	D	279	LYS	2.4
1	C	21	THR	2.4
1	A	193	ALA	2.3
1	D	311	ARG	2.3
1	C	312	LYS	2.3
1	D	269	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	276	LEU	2.2
1	C	157	VAL	2.2
1	B	278	LYS	2.2
1	B	311	ARG	2.2
1	C	300	CYS	2.1
1	B	194	GLU	2.1
1	B	68	ILE	2.1
1	D	225	ARG	2.1
1	D	259	ASN	2.1
1	A	186	GLU	2.1
1	B	20	LYS	2.1
1	D	296	ILE	2.1
1	B	308	MET	2.1
1	C	69	LYS	2.1
1	D	106	GLU	2.1
1	A	20	LYS	2.0
1	A	40	LYS	2.0
1	B	294	LYS	2.0
1	D	23	THR	2.0
1	A	91	PRO	2.0
1	D	91	PRO	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.