



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:31 AM GMT

PDB ID : 3EYI  
Title : The crystal structure of the second Z-DNA binding domain of human DAI (ZBP1) in complex with Z-DNA  
Authors : Ha, S.C.; Kim, K.K.  
Deposited on : 2008-10-21  
Resolution : 1.45 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

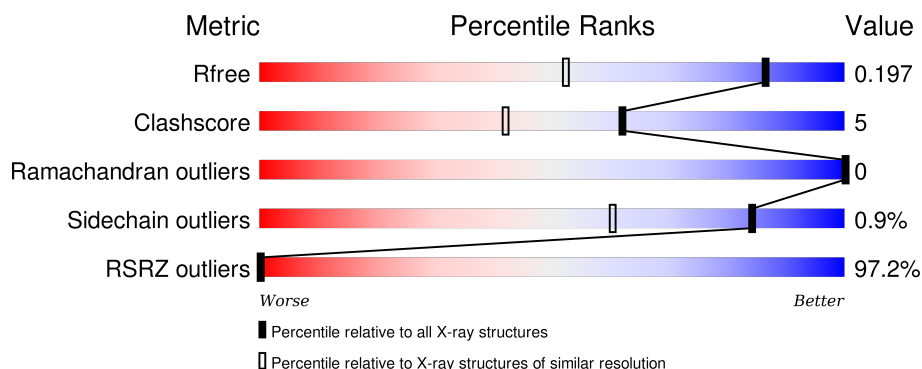
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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	72	
1	B	72	
2	C	7	
2	D	7	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1707 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 Z-DNA-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			535	333	100	99	3			
1	B	67	Total	C	N	O	S	0	0	0
			558	347	105	102	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP Q9H171
A	-3	MET	-	EXPRESSION TAG	UNP Q9H171
A	-2	ALA	-	EXPRESSION TAG	UNP Q9H171
A	-1	SER	-	EXPRESSION TAG	UNP Q9H171
A	167	TRP	-	EXPRESSION TAG	UNP Q9H171
A	168	THR	-	EXPRESSION TAG	UNP Q9H171
A	169	ILE	-	EXPRESSION TAG	UNP Q9H171
A	170	TYR	-	EXPRESSION TAG	UNP Q9H171
B	-4	HIS	-	EXPRESSION TAG	UNP Q9H171
B	-3	MET	-	EXPRESSION TAG	UNP Q9H171
B	-2	ALA	-	EXPRESSION TAG	UNP Q9H171
B	-1	SER	-	EXPRESSION TAG	UNP Q9H171
B	167	TRP	-	EXPRESSION TAG	UNP Q9H171
B	168	THR	-	EXPRESSION TAG	UNP Q9H171
B	169	ILE	-	EXPRESSION TAG	UNP Q9H171
B	170	TYR	-	EXPRESSION TAG	UNP Q9H171

- Molecule 2 is a DNA chain called 5'-TCGCGCG-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			123	57	24	36	6			
2	D	7	Total	C	N	O	P	0	0	0
			140	67	26	41	6			

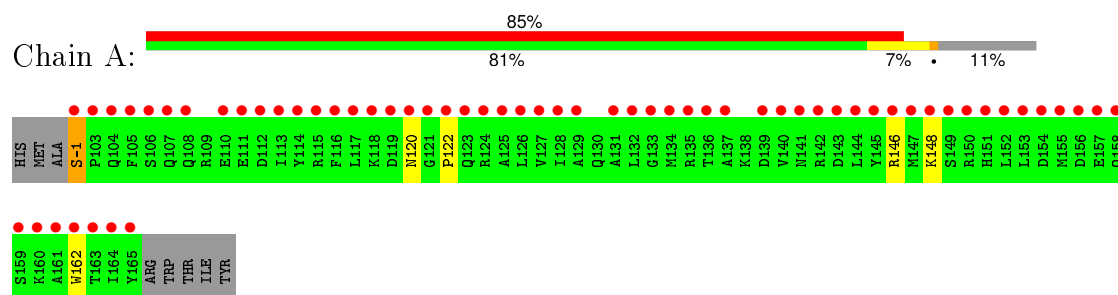
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total 129	O 129	0	0
3	B	129	Total 129	O 129	0	0
3	C	43	Total 43	O 43	0	0
3	D	50	Total 50	O 50	0	0

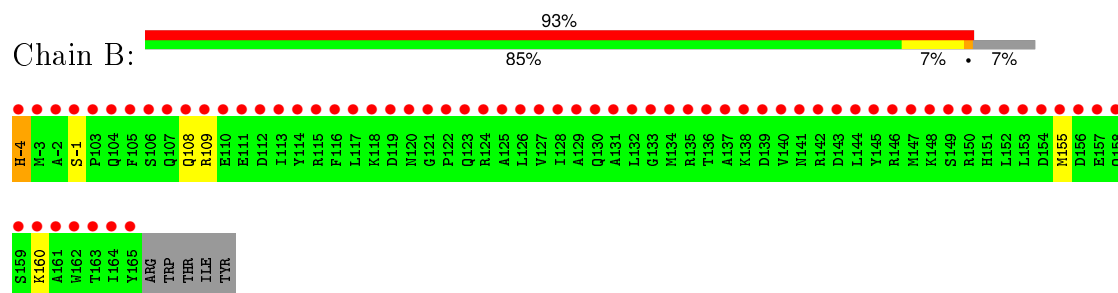
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

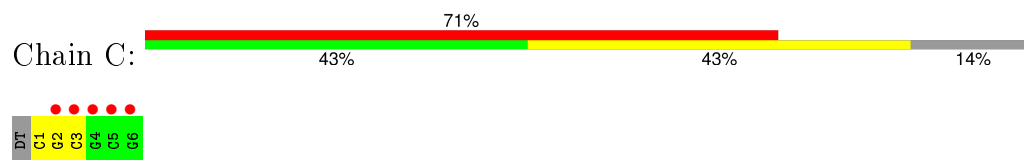
#### • Molecule 1: Z-DNA-binding protein 1



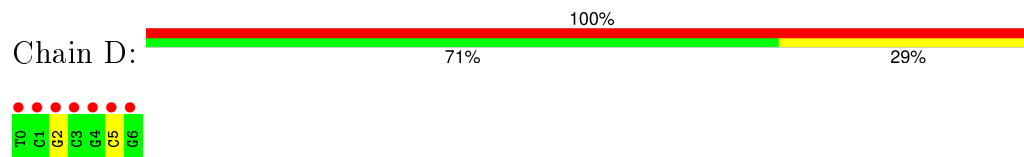
#### • Molecule 1: Z-DNA-binding protein 1



#### • Molecule 2: 5'-TCGCGCG-3'



#### • Molecule 2: 5'-TCGCGCG-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	29.53Å 58.25Å 88.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.45 18.97 – 1.45	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-1.45) 94.7 (18.97-1.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.153 , 0.194 0.158 , 0.197	Depositor DCC
$R_{free}$ test set	2617 reflections (10.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	1.6	Xtriage
Anisotropy	0.921	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 26421 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.59% 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	0.90	1/544 (0.2%)	0.90	0/729
1	B	0.90	1/568 (0.2%)	0.99	2/761 (0.3%)
2	C	1.32	0/137	1.94	4/209 (1.9%)
2	D	1.23	0/156	1.78	3/239 (1.3%)
All	All	0.99	2/1405 (0.1%)	1.22	9/1938 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-1	SER	C-N	13.36	1.59	1.34
1	B	-1	SER	C-N	12.94	1.58	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	B	109	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	C	2	DG	C4-C5-N7	6.43	113.37	110.80
2	C	1	DC	C5-C6-N1	-6.14	117.93	121.00
2	D	2	DG	O4'-C1'-N9	-6.13	103.71	108.00
2	D	5	DC	C5-C4-N4	5.83	124.28	120.20
2	C	1	DC	O5'-P-OP2	-5.72	100.55	105.70
2	C	3	DC	C5-C6-N1	-5.60	118.20	121.00
2	D	5	DC	N3-C4-C5	-5.32	119.77	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	SER	Mainchain

## 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	535	0	532	4	0
1	B	558	0	553	10	0
2	C	123	0	67	0	0
2	D	140	0	80	0	0
3	A	129	0	0	3	1
3	B	129	0	0	9	1
3	C	43	0	0	0	0
3	D	50	0	0	1	0
All	All	1707	0	1232	14	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 5.

All (14) 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:155:MET:CG	3:B:362:HOH:O	1.90	1.15
1:B:155:MET:CE	3:B:362:HOH:O	1.96	1.13
1:B:155:MET:HE2	3:B:362:HOH:O	1.53	0.99
1:B:155:MET:HG2	3:B:362:HOH:O	1.51	0.99
1:B:155:MET:SD	3:B:362:HOH:O	2.20	0.97
1:A:146:ARG:NH2	3:A:367:HOH:O	2.14	0.79
1:B:160:LYS:HD3	3:D:170:HOH:O	1.85	0.77
1:B:-4:HIS:N	3:B:201:HOH:O	2.28	0.66
1:A:120:ASN:OD1	3:A:366:HOH:O	2.17	0.59
1:A:122:PRO:HA	1:A:162:TRP:O	2.12	0.49
1:B:108:GLN:HG2	3:B:369:HOH:O	2.17	0.44
1:B:-4:HIS:N	3:B:364:HOH:O	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-4:HIS:CA	3:B:364:HOH:O	2.53	0.43
1:A:148:LYS:NZ	3:A:280:HOH:O	2.53	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)
3:A:53:HOH:O	3:B:369:HOH:O[4_565]	1.79	0.41

## 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	62/72 (86%)	60 (97%)	2 (3%)	0	100	100
1	B	65/72 (90%)	63 (97%)	2 (3%)	0	100	100
All	All	127/144 (88%)	123 (97%)	4 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	57/64 (89%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	59/64 (92%)	58 (98%)	1 (2%)	68	32
All	All	116/128 (91%)	115 (99%)	1 (1%)	84	60

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	-4	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	B	107	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	64/72 (88%)	4.29	61 (95%)  	7, 13, 23, 31	0
1	B	67/72 (93%)	4.06	67 (100%)  	7, 12, 19, 26	0
2	C	6/7 (85%)	2.33	5 (83%)  	7, 8, 10, 13	0
2	D	7/7 (100%)	2.71	7 (100%)  	7, 8, 9, 20	0
All	All	144/158 (91%)	4.02	140 (97%)  	7, 12, 21, 31	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	16.8
1	B	164	ILE	9.4
1	A	165	TYR	8.9
1	A	127	VAL	8.1
1	A	132	LEU	7.8
1	B	165	TYR	6.8
1	B	162	TRP	6.8
1	B	113	ILE	6.7
1	B	121	GLY	6.5
1	B	127	VAL	6.4
1	B	125	ALA	6.3
1	A	113	ILE	6.2
1	A	162	TRP	6.2
1	A	157	GLU	6.1
1	A	105	PHE	6.1
1	A	106	SER	6.0
1	B	105	PHE	6.0
1	A	116	PHE	5.9
1	B	115	ARG	5.9
1	B	132	LEU	5.9
1	B	160	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	144	LEU	5.8
1	B	129	ALA	5.5
1	A	140	VAL	5.5
1	B	114	TYR	5.5
1	A	-1	SER	5.5
1	A	146	ARG	5.4
1	B	122	PRO	5.3
1	B	126	LEU	5.3
1	B	-2	ALA	5.3
1	A	144	LEU	5.2
1	B	140	VAL	5.1
1	B	145	TYR	5.1
1	B	109	ARG	5.1
1	A	152	LEU	5.0
1	B	116	PHE	4.9
1	A	136	THR	4.8
1	B	152	LEU	4.8
1	B	153	LEU	4.7
1	B	150	ARG	4.7
1	A	159	SER	4.7
1	A	145	TYR	4.7
1	A	163	THR	4.6
1	A	114	TYR	4.6
1	A	129	ALA	4.6
1	B	118	LYS	4.6
1	A	108	GLN	4.6
1	A	128	ILE	4.5
1	B	-3	MET	4.5
1	A	104	GLN	4.5
1	A	164	ILE	4.5
1	A	153	LEU	4.4
1	A	147	MET	4.4
1	B	131	ALA	4.4
1	B	158	GLN	4.4
1	A	121	GLY	4.1
1	A	160	LYS	4.1
1	A	161	ALA	4.1
1	A	117	LEU	4.1
1	B	128	ILE	4.0
1	A	148	LYS	4.0
1	A	158	GLN	4.0
1	A	107	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	149	SER	4.0
1	B	-4	HIS	3.9
1	B	136	THR	3.9
1	B	124	ARG	3.9
1	A	112	ASP	3.9
1	B	157	GLU	3.8
1	B	117	LEU	3.8
1	A	154	ASP	3.7
1	A	115	ARG	3.7
1	A	103	PRO	3.7
1	B	134	MET	3.7
1	A	125	ALA	3.4
1	B	161	ALA	3.4
1	A	131	ALA	3.4
1	A	142	ARG	3.4
1	B	137	ALA	3.3
1	B	156	ASP	3.2
1	A	137	ALA	3.2
1	A	155	MET	3.2
1	B	142	ARG	3.2
1	B	133	GLY	3.2
1	B	143	ASP	3.2
2	D	0	DT	3.1
1	B	130	GLN	3.1
1	A	111	GLU	3.0
1	A	122	PRO	3.0
1	B	163	THR	3.0
1	A	120	ASN	3.0
1	B	151	HIS	3.0
1	B	-1	SER	3.0
1	A	143	ASP	3.0
1	A	124	ARG	3.0
1	B	119	ASP	3.0
1	A	151	HIS	3.0
2	D	5	DC	3.0
1	A	150	ARG	3.0
1	B	106	SER	2.9
1	A	118	LYS	2.9
1	B	146	ARG	2.9
1	A	156	ASP	2.9
1	B	155	MET	2.8
1	B	107	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	103	PRO	2.8
2	D	6	DG	2.8
1	B	139	ASP	2.8
1	A	134	MET	2.7
1	B	111	GLU	2.7
2	D	3	DC	2.7
2	D	2	DG	2.7
1	B	141	ASN	2.7
1	B	112	ASP	2.6
1	B	108	GLN	2.6
1	B	154	ASP	2.6
1	A	119	ASP	2.6
1	A	133	GLY	2.6
2	C	4	DG	2.6
1	B	123	GLN	2.6
1	B	149	SER	2.5
1	B	148	LYS	2.5
1	A	141	ASN	2.5
2	C	2	DG	2.5
2	C	5	DC	2.4
2	C	6	DG	2.4
2	D	4	DG	2.4
1	B	159	SER	2.3
2	D	1	DC	2.3
2	C	3	DC	2.3
1	A	135	ARG	2.3
1	B	120	ASN	2.2
1	A	110	GLU	2.1
1	B	135	ARG	2.1
1	B	138	LYS	2.1
1	A	139	ASP	2.1
1	B	104	GLN	2.0
1	B	147	MET	2.0
1	A	123	GLN	2.0
1	B	110	GLU	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.