



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:11 AM GMT

PDB ID : 3K3R  
Title : Unrefined crystal structure of a LexA-DNA complex  
Authors : Zhang, A.P.P.; Pigli, Y.Z.; Rice, P.A.  
Deposited on : 2009-10-04  
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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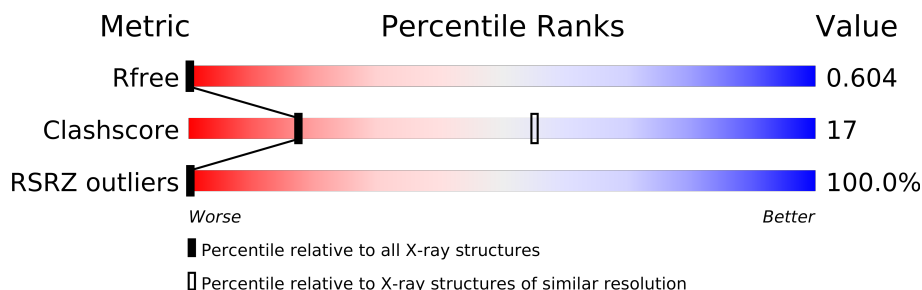
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance




The reported resolution of this entry is 3.20 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	202	
1	F	202	
2	A	29	
2	B	29	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 403 atoms, of which 0 are hydrogen and 0 are deuterium.

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 LexA repressor.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	E	174	Total C 174 174	0	0	174
1	F	173	Total C 173 173	0	0	173

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	156	ALA	LYS	ENGINEERED	UNP P0A7C2
F	156	ALA	LYS	ENGINEERED	UNP P0A7C2

- Molecule 2 is a DNA chain called DNA (28-MER).

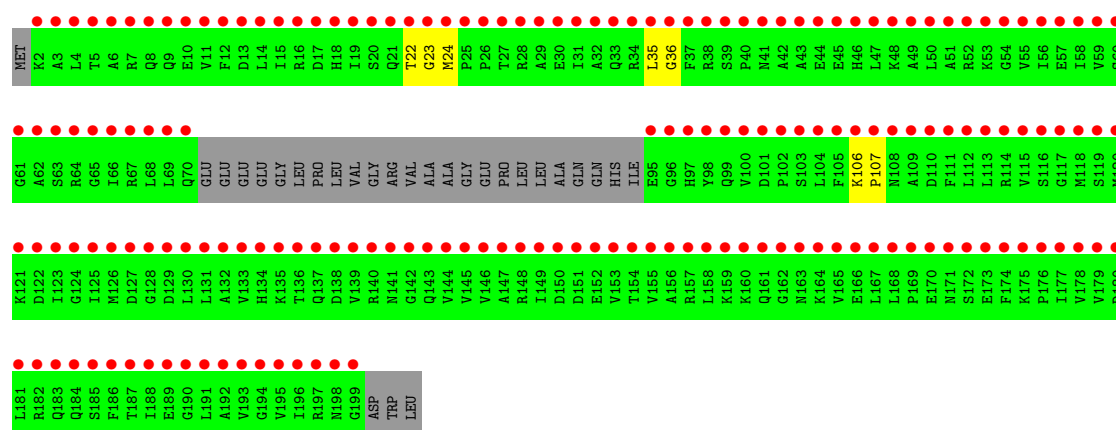
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	A	28	Total P 28 28	0	0	28
2	B	28	Total P 28 28	0	0	28

### 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.

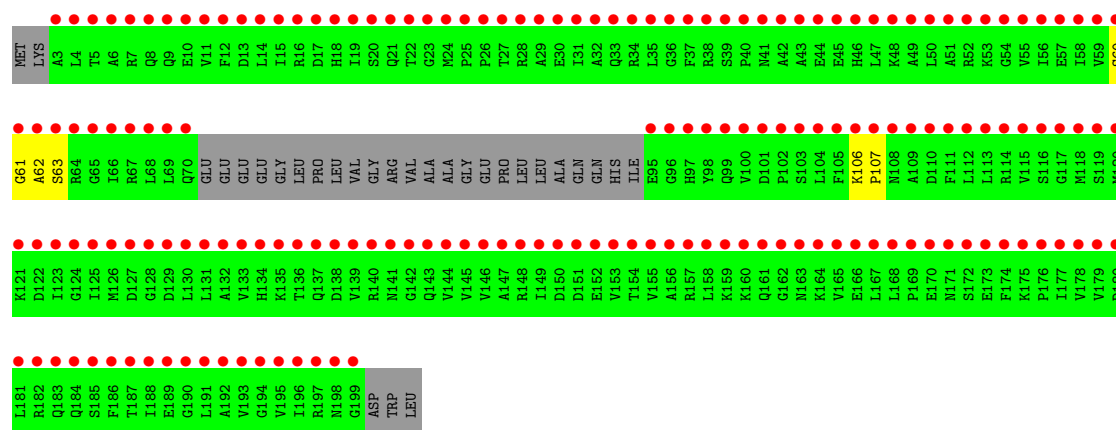
- Molecule 1: LexA repressor

Chain E: 



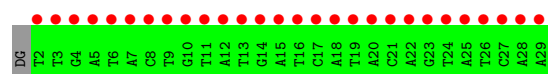
- Molecule 1: LexA repressor

Chain F: 

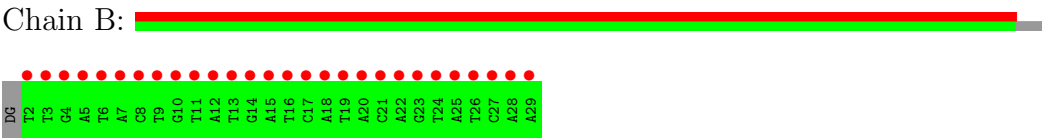


- Molecule 2: DNA (28-MER)

Chain A: 



- Molecule 2: DNA (28-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.36 Å 120.39 Å 149.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 35.76 – 3.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.20) 95.7 (35.76-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.18 Å)	Xtriage
Refinement program	?	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.604 , 0.604	Depositor DCC
$R_{free}$ test set	688 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.66 , 63.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 13754 reflections	Xtriage
$F_o, F_c$ correlation	0.69	EDS
Total number of atoms	403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	$\# Z  > 5$

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	174	0	0	4	0
1	F	173	0	0	3	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
All	All	403	0	0	7	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:60:SER:CA	1:F:61:GLY:CA	2.78	0.60
1:F:106:LYS:CA	1:F:107:PRO:CA	2.86	0.53
1:E:22:THR:CA	1:E:23:GLY:CA	2.88	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:23:GLY:CA	1:E:24:MET:CA	2.90	0.50
1:E:35:LEU:CA	1:E:36:GLY:CA	2.91	0.49
1:F:62:ALA:CA	1:F:63:SER:CA	2.91	0.48
1:E:106:LYS:CA	1:E:107:PRO:CA	2.99	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

There are no RNA chains 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	E	174/202 (86%)	21.23	174 (100%) <b>0</b> <b>0</b>	26, 137, 137, 137	0
1	F	173/202 (85%)	22.75	173 (100%) <b>0</b> <b>0</b>	137, 137, 137, 137	0
2	A	28/29 (96%)	13.10	28 (100%) <b>0</b> <b>0</b>	119, 119, 119, 119	0
2	B	28/29 (96%)	15.68	28 (100%) <b>0</b> <b>0</b>	119, 119, 119, 119	0
All	All	403/462 (87%)	20.93	403 (100%) <b>0</b> <b>0</b>	26, 137, 137, 137	0

All (403) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	123	ILE	55.9
1	F	181	LEU	49.0
1	F	108	ASN	47.9
1	E	182	ARG	47.4
1	E	118	MET	46.5
1	E	14	LEU	45.4
1	E	183	GLN	45.3
1	E	95	GLU	44.7
1	E	70	GLN	44.0
1	E	152	GLU	43.8
1	E	142	GLY	43.6
1	F	169	PRO	43.5
1	E	177	ILE	43.4
1	E	181	LEU	43.3
1	E	106	LYS	43.1
1	E	24	MET	42.9
1	F	199	GLY	42.5
1	F	48	LYS	41.5
1	E	57	GLU	41.3
1	E	163	ASN	39.8
1	F	99	GLN	39.3

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Mol	Chain	Res	Type	RSRZ
1	F	107	PRO	39.3
1	F	9	GLN	39.3
1	F	57	GLU	38.7
1	E	107	PRO	38.3
1	F	109	ALA	37.5
1	E	161	GLN	37.4
1	E	171	ASN	36.0
1	E	169	PRO	36.0
1	F	66	ILE	35.8
1	F	58	ILE	35.4
1	F	191	LEU	35.3
1	E	144	VAL	35.1
1	F	187	THR	35.0
1	E	170	GLU	35.0
1	F	62	ALA	34.7
1	E	179	VAL	34.5
1	F	56	ILE	34.0
1	F	163	ASN	33.6
1	F	68	LEU	33.4
1	F	141	ASN	33.3
1	F	60	SER	33.2
1	F	150	ASP	33.0
1	F	127	ASP	32.8
1	F	115	VAL	32.5
1	F	39	SER	32.5
1	E	136	THR	32.1
1	F	161	GLN	31.8
1	E	38	ARG	31.8
1	E	15	ILE	31.4
1	E	160	LYS	31.2
1	F	95	GLU	31.0
1	F	159	LYS	30.4
1	E	123	ILE	30.3
1	F	172	SER	29.9
1	F	45	GLU	29.8
1	F	54	GLY	29.7
1	F	7	ARG	29.5
1	F	130	LEU	29.5
1	F	5	THR	29.5
1	E	197	ARG	29.1
1	F	101	ASP	28.8
1	F	35	LEU	28.7

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Mol	Chain	Res	Type	RSRZ
1	F	184	GLN	28.6
1	F	197	ARG	28.3
1	F	146	VAL	28.3
1	F	38	ARG	28.2
1	E	138	ASP	28.1
1	F	51	ALA	28.1
1	F	70	GLN	28.1
1	F	168	LEU	28.0
1	F	190	GLY	27.5
2	A	11	DT	27.5
1	E	184	GLN	27.3
1	F	162	GLY	27.2
1	F	134	HIS	27.1
1	F	149	ILE	27.1
1	F	22	THR	27.0
1	F	157	ARG	27.0
1	E	28	ARG	26.9
1	E	162	GLY	26.8
1	F	98	TYR	26.8
1	E	53	LYS	26.8
1	E	143	GLN	26.6
1	E	157	ARG	26.5
1	F	10	GLU	26.5
2	B	25	DA	26.4
1	F	53	LYS	26.3
1	E	134	HIS	26.2
1	E	164	LYS	26.2
1	E	175	LYS	26.1
1	F	158	LEU	26.1
1	F	136	THR	26.0
1	F	114	ARG	26.0
1	F	164	LYS	25.9
1	E	198	ASN	25.7
1	F	47	LEU	25.7
1	F	140	ARG	25.4
1	E	174	PHE	25.3
1	F	142	GLY	25.2
1	F	180	ASP	25.2
1	E	58	ILE	25.2
1	E	35	LEU	25.2
1	E	67	ARG	25.1
1	F	59	VAL	25.1

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Mol	Chain	Res	Type	RSRZ
1	F	126	MET	24.6
1	F	46	HIS	24.6
1	E	167	LEU	24.6
1	E	6	ALA	24.5
1	E	117	GLY	24.4
1	E	66	ILE	24.4
1	F	106	LYS	24.4
1	F	55	VAL	24.4
1	F	49	ALA	24.4
1	F	26	PRO	24.1
1	E	27	THR	24.1
1	F	37	PHE	23.9
1	F	122	ASP	23.8
1	E	56	ILE	23.7
1	F	8	GLN	23.7
1	F	61	GLY	23.6
1	F	111	PHE	23.5
1	F	21	GLN	23.4
1	E	114	ARG	23.4
1	F	67	ARG	23.3
1	F	125	ILE	23.2
2	B	7	DA	23.2
1	F	173	GLU	23.2
1	E	185	SER	23.2
1	F	118	MET	23.2
1	F	14	LEU	23.2
1	F	170	GLU	23.1
1	E	141	ASN	23.1
1	E	126	MET	23.0
1	E	55	VAL	22.9
1	F	147	ALA	22.8
1	E	17	ASP	22.7
1	F	20	SER	22.6
1	F	33	GLN	22.6
1	E	192	ALA	22.5
1	F	151	ASP	22.5
2	B	18	DA	22.4
1	E	158	LEU	22.4
1	F	100	VAL	22.3
1	F	117	GLY	22.3
1	F	23	GLY	22.1
1	E	129	ASP	22.1

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Mol	Chain	Res	Type	RSRZ
1	E	137	GLN	22.1
1	E	122	ASP	22.0
1	F	176	PRO	22.0
1	E	109	ALA	22.0
1	F	16	ARG	21.8
1	F	63	SER	21.8
1	F	132	ALA	21.8
1	E	193	VAL	21.6
1	F	148	ARG	21.6
1	E	26	PRO	21.4
1	E	111	PHE	21.4
1	F	96	GLY	21.3
1	E	33	GLN	21.3
1	F	104	LEU	21.3
1	E	180	ASP	21.2
1	F	36	GLY	21.1
1	E	186	PHE	21.1
1	E	199	GLY	21.1
1	F	65	GLY	20.8
1	E	116	SER	20.8
1	F	40	PRO	20.7
1	E	101	ASP	20.7
1	E	178	VAL	20.6
1	E	172	SER	20.5
1	E	54	GLY	20.4
1	F	171	ASN	20.4
1	F	189	GLU	20.3
1	E	52	ARG	20.2
1	F	34	ARG	20.1
1	E	145	VAL	20.0
1	E	63	SER	20.0
1	F	3	ALA	20.0
2	B	21	DC	20.0
1	E	31	ILE	19.8
2	B	20	DA	19.8
1	F	186	PHE	19.7
1	E	62	ALA	19.6
1	F	31	ILE	19.5
2	B	16	DT	19.5
1	F	15	ILE	19.5
2	B	15	DA	19.4
1	E	5	THR	19.4

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Mol	Chain	Res	Type	RSRZ
1	E	156	ALA	19.3
1	E	68	LEU	19.3
1	F	179	VAL	19.3
1	F	152	GLU	19.2
1	E	97	HIS	19.2
1	E	69	LEU	19.2
1	F	110	ASP	19.1
1	E	176	PRO	19.1
1	E	13	ASP	19.0
1	F	18	HIS	19.0
1	E	125	ILE	18.9
1	E	149	ILE	18.8
1	E	108	ASN	18.8
1	F	50	LEU	18.7
1	E	45	GLU	18.6
1	E	96	GLY	18.6
1	E	16	ARG	18.5
1	F	167	LEU	18.5
2	B	12	DA	18.4
2	B	22	DA	18.3
1	E	25	PRO	18.3
1	F	97	HIS	18.2
1	E	48	LYS	18.2
1	F	102	PRO	18.1
2	B	23	DG	18.1
1	E	4	LEU	18.1
1	E	153	VAL	18.1
1	E	102	PRO	18.0
1	E	196	ILE	18.0
1	E	135	LYS	18.0
1	E	191	LEU	18.0
1	F	124	GLY	17.9
1	F	182	ARG	17.8
1	F	195	VAL	17.8
1	F	145	VAL	17.8
1	F	24	MET	17.8
1	F	27	THR	17.7
1	E	47	LEU	17.7
1	E	165	VAL	17.7
1	E	168	LEU	17.7
1	E	99	GLN	17.6
1	F	135	LYS	17.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	147	ALA	17.6
1	F	121	LYS	17.6
1	F	120	MET	17.6
1	F	183	GLN	17.6
2	B	6	DT	17.5
1	E	21	GLN	17.5
1	E	173	GLU	17.5
1	F	128	GLY	17.5
1	F	105	PHE	17.5
1	F	52	ARG	17.5
1	F	175	LYS	17.4
1	E	20	SER	17.2
1	F	129	ASP	17.2
1	F	188	ILE	17.2
1	E	60	SER	17.2
1	F	19	ILE	17.2
1	E	49	ALA	17.1
1	E	51	ALA	17.1
1	F	17	ASP	17.0
1	F	41	ASN	17.0
1	E	139	VAL	17.0
1	E	120	MET	16.9
1	F	112	LEU	16.8
1	E	150	ASP	16.8
2	A	7	DA	16.8
2	A	20	DA	16.8
1	E	133	VAL	16.6
2	A	19	DT	16.6
1	F	28	ARG	16.5
1	F	138	ASP	16.5
1	E	39	SER	16.5
1	F	137	GLN	16.3
1	E	7	ARG	16.3
1	E	132	ALA	16.3
2	B	17	DC	16.3
1	F	143	GLN	16.2
1	E	29	ALA	16.2
2	A	16	DT	16.2
1	E	32	ALA	16.1
1	F	198	ASN	16.0
1	E	115	VAL	15.9
2	A	15	DA	15.9

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Mol	Chain	Res	Type	RSRZ
1	E	113	LEU	15.9
1	E	124	GLY	15.9
1	E	41	ASN	15.8
1	E	155	VAL	15.7
1	F	103	SER	15.7
2	A	6	DT	15.7
1	F	174	PHE	15.7
1	E	104	LEU	15.6
2	B	14	DG	15.6
1	E	146	VAL	15.6
1	E	8	GLN	15.6
1	E	110	ASP	15.6
1	E	10	GLU	15.6
1	E	128	GLY	15.5
1	E	23	GLY	15.4
1	E	98	TYR	15.4
1	F	64	ARG	15.3
2	B	26	DT	15.1
1	F	156	ALA	15.0
1	F	185	SER	15.0
1	E	127	ASP	15.0
1	E	100	VAL	15.0
2	A	9	DT	14.9
1	E	40	PRO	14.9
2	B	28	DA	14.8
1	E	19	ILE	14.8
1	E	154	THR	14.7
1	F	160	LYS	14.6
1	F	29	ALA	14.6
1	F	42	ALA	14.6
1	E	22	THR	14.6
1	E	18	HIS	14.6
1	E	30	GLU	14.5
2	B	8	DC	14.5
1	E	59	VAL	14.4
1	E	36	GLY	14.4
1	F	194	GLY	14.3
1	E	119	SER	14.3
1	E	187	THR	14.3
1	E	61	GLY	14.3
1	F	25	PRO	14.3
1	F	13	ASP	14.2

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Mol	Chain	Res	Type	RSRZ
1	E	148	ARG	14.1
1	E	105	PHE	14.1
1	E	121	LYS	14.1
2	A	10	DG	14.1
2	A	14	DG	14.1
1	E	37	PHE	14.0
1	F	196	ILE	13.9
2	A	5	DA	13.9
2	A	28	DA	13.8
2	B	4	DG	13.8
2	B	10	DG	13.8
1	F	30	GLU	13.7
1	F	119	SER	13.7
1	F	177	ILE	13.7
1	F	133	VAL	13.6
1	E	188	ILE	13.6
1	F	32	ALA	13.6
1	E	65	GLY	13.6
1	E	189	GLU	13.5
2	A	18	DA	13.5
2	B	3	DT	13.3
2	B	9	DT	13.3
1	E	46	HIS	13.2
1	E	9	GLN	13.2
1	F	113	LEU	13.2
1	E	34	ARG	13.0
1	F	178	VAL	13.0
2	A	21	DC	12.9
1	F	131	LEU	12.8
1	F	12	PHE	12.8
1	F	166	GLU	12.8
2	B	5	DA	12.7
2	A	17	DC	12.7
1	E	166	GLU	12.7
1	E	190	GLY	12.7
2	A	4	DG	12.6
1	F	43	ALA	12.6
1	F	139	VAL	12.6
1	E	3	ALA	12.5
1	E	43	ALA	12.5
1	E	42	ALA	12.4
1	E	130	LEU	12.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	140	ARG	12.4
2	B	11	DT	12.1
1	F	144	VAL	12.1
2	A	13	DT	12.0
1	E	112	LEU	11.9
1	E	159	LYS	11.9
2	B	29	DA	11.9
2	A	22	DA	11.8
1	E	151	ASP	11.8
1	F	165	VAL	11.8
1	F	44	GLU	11.6
2	A	2	DT	11.2
1	F	11	VAL	11.1
1	E	44	GLU	11.0
1	F	193	VAL	11.0
2	A	29	DA	10.9
1	E	131	LEU	10.9
2	A	24	DT	10.8
1	F	155	VAL	10.7
2	A	12	DA	10.6
2	A	25	DA	10.6
2	B	19	DT	10.6
1	F	69	LEU	10.5
1	E	50	LEU	10.4
2	A	26	DT	10.3
2	B	27	DC	10.1
1	F	6	ALA	10.0
1	E	194	GLY	10.0
2	B	2	DT	9.9
1	F	153	VAL	9.8
2	B	13	DT	9.8
1	E	12	PHE	9.7
1	F	192	ALA	9.5
1	F	154	THR	9.4
1	F	116	SER	9.4
1	E	103	SER	9.1
1	E	2	LYS	9.0
1	E	11	VAL	8.9
2	A	23	DG	8.5
2	B	24	DT	8.2
2	A	27	DC	8.1
2	A	8	DC	8.1

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Mol	Chain	Res	Type	RSRZ
1	E	64	ARG	7.8
1	E	195	VAL	7.5
1	F	4	LEU	6.4
2	A	3	DT	6.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.