



# wwPDB X-ray Structure Validation Summary Report

Mar 17, 2026 – 11:37 PM UTC

PDB ID : 6LA2 / pdb\_00006la2  
Title : 343 bp di-nucleosome harboring cohesive DNA termini assembled with linker histone H1.0  
Authors : Adhireksan, Z.; Sharma, D.; Lee, P.L.; Davey, C.A.  
Deposited on : 2019-11-11  
Resolution : 3.89 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

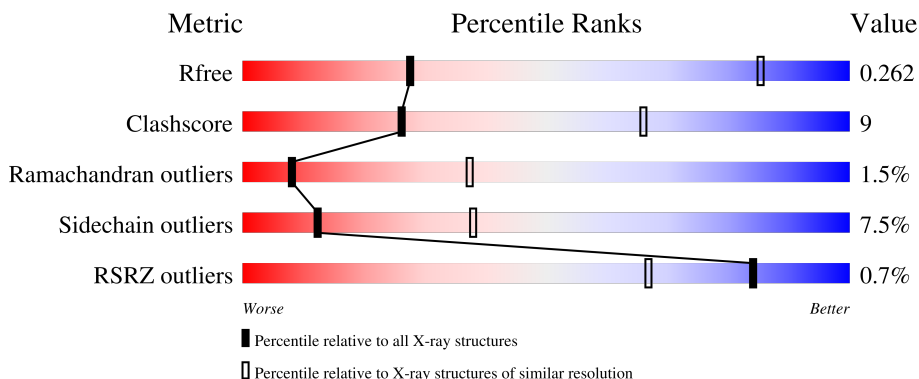
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.89 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.







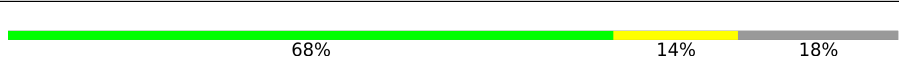
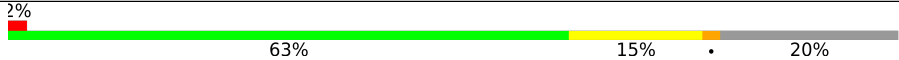
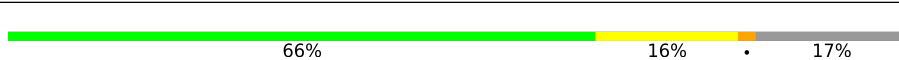
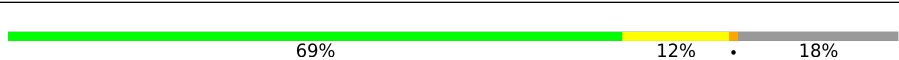
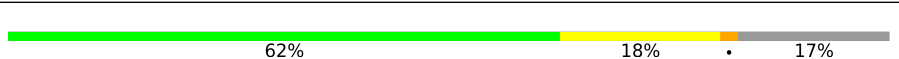
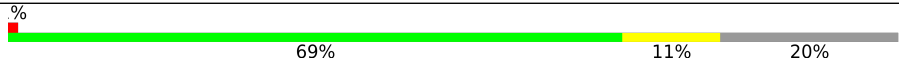
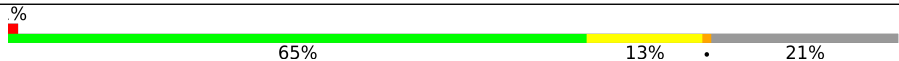
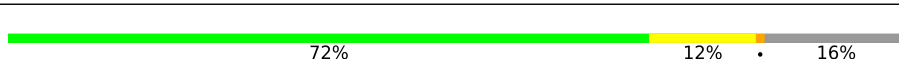


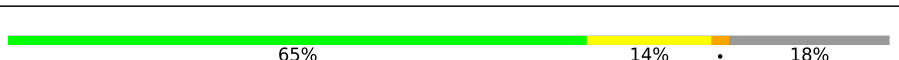
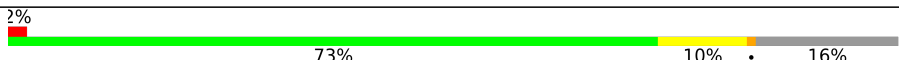
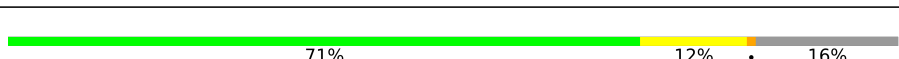
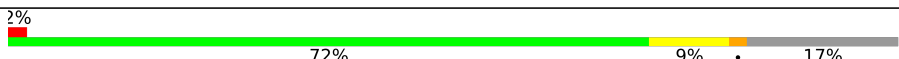






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	136	 57% 15% 26%
1	E	136	 60% 12% 26%
1	K	136	 60% 12% 27%
1	O	136	 63% 9% 27%
1	U	136	 62% 10% 27%









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Mol	Chain	Length	Quality of chain
1	Y	136	 % 63% 10% 26%
1	e	136	 4% 60% 12% 27%
1	i	136	 % 62% 11% 26%
2	B	103	 66% 13% 19%
2	F	103	 68% 14% 18%
2	L	103	 2% 63% 15% 20%
2	P	103	 66% 16% 17%
2	V	103	 69% 12% 18%
2	Z	103	 62% 18% 17%
2	f	103	 % 69% 11% 20%
2	j	103	 % 65% 13% 21%
3	C	130	 72% 12% 16%
3	G	130	 68% 11% 20%
3	M	130	 72% 12% 16%
3	Q	130	 65% 14% 18%
3	W	130	 2% 73% 10% 16%
3	a	130	 67% 12% 21%
3	g	130	 71% 12% 16%
3	k	130	 2% 72% 9% 17%
4	D	126	 52% 22% 23%
4	H	126	 % 53% 20% 24%
4	N	126	 % 51% 23% 23%
4	R	126	 % 49% 24% 24%
4	X	126	 2% 48% 22% 28%
4	b	126	 % 50% 23% 24%

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Mol	Chain	Length	Quality of chain
4	h	126	
4	l	126	
5	I	343	
5	c	343	
6	J	343	
6	d	343	
7	S	194	
7	T	194	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 53828 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 Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	e	99	816	514	158	140	4	0	0	0
1	i	100	825	520	160	141	4	0	0	0
1	A	100	825	520	160	141	4	0	0	0
1	E	100	825	520	160	141	4	0	0	0
1	K	99	816	514	158	140	4	0	0	0
1	O	99	816	514	158	140	4	0	0	0
1	U	99	816	514	158	140	4	0	0	0
1	Y	100	825	520	160	141	4	0	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	f	82	653	412	127	113	1	0	0	0
2	j	81	646	407	126	112	1	0	0	0
2	B	83	662	418	129	114	1	0	0	0
2	F	84	673	424	133	115	1	0	0	0
2	L	82	653	412	127	113	1	0	0	0
2	P	86	694	436	140	117	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			
2	Z	85	Total	C	N	O	S	0	0	0
			683	430	136	116	1			

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	g	109	Total	C	N	O	0	0	0
			844	532	167	145			
3	k	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	C	109	Total	C	N	O	0	0	0
			844	532	167	145			
3	G	104	Total	C	N	O	0	0	0
			805	508	157	140			
3	M	109	Total	C	N	O	0	0	0
			844	532	167	145			
3	Q	106	Total	C	N	O	0	0	0
			819	517	160	142			
3	W	109	Total	C	N	O	0	0	0
			844	532	167	145			
3	a	103	Total	C	N	O	0	0	0
			796	502	155	139			

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	h	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	l	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	D	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			
4	H	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	N	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			
4	R	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	X	91	Total	C	N	O	S	0	0	0
			709	447	125	135	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	b	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

- Molecule 5 is a DNA chain called DNA (343-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	343	Total	C	N	O	P	0	0	0
			7024	3330	1329	2022	343			
5	c	343	Total	C	N	O	P	0	0	0
			7024	3330	1329	2022	343			

- Molecule 6 is a DNA chain called DNA (343-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	343	Total	C	N	O	P	0	0	0
			7041	3348	1254	2096	343			
6	d	343	Total	C	N	O	P	0	0	0
			7041	3348	1254	2096	343			

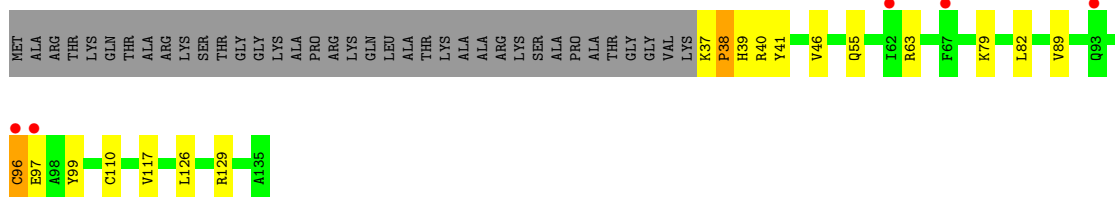
- Molecule 7 is a protein called Histone H1.0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S	75	Total	C	N	O	S	0	0	0
			575	358	108	108	1			
7	T	75	Total	C	N	O	S	0	0	0
			575	358	108	108	1			

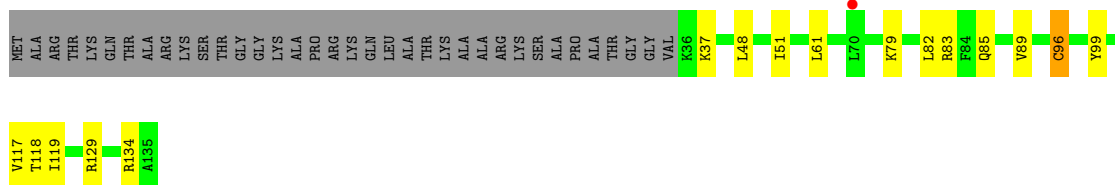
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

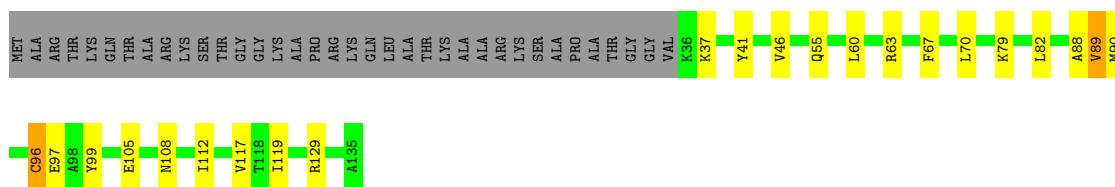
- Molecule 1: Histone H3.1



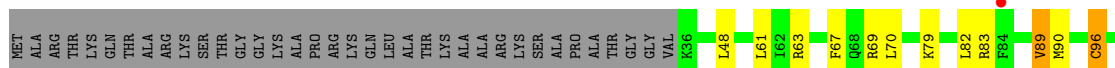
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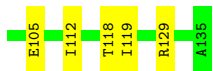
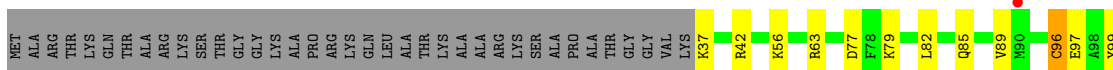


- Molecule 1: Histone H3.1

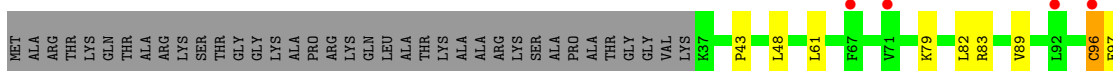




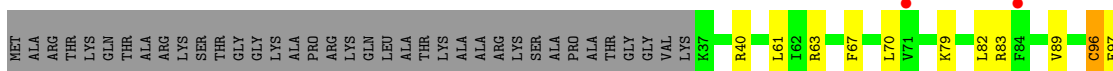
- Molecule 1: Histone H3.1



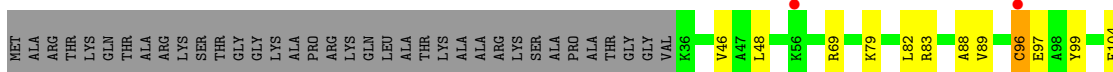
- Molecule 1: Histone H3.1



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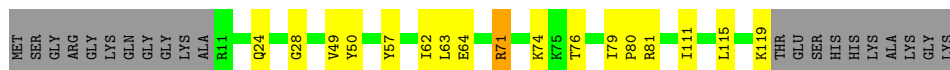
- Molecule 2: Histone H4







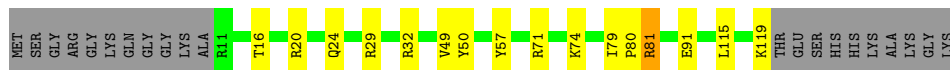
- Molecule 3: Histone H2A type 1-B/E



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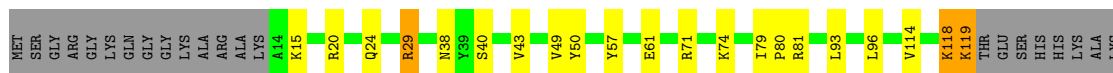
- Molecule 3: Histone H2A type 1-B/E



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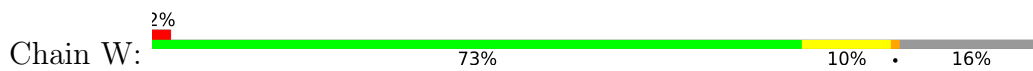


- Molecule 3: Histone H2A type 1-B/E



GLY  
LYS

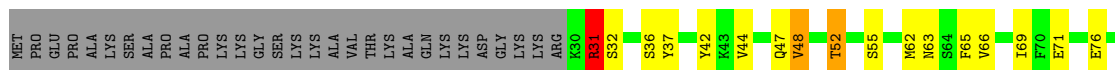
- Molecule 3: Histone H2A type 1-B/E



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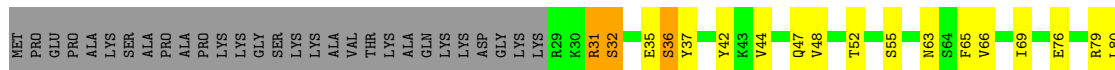
• Molecule 4: Histone H2B type 1-J



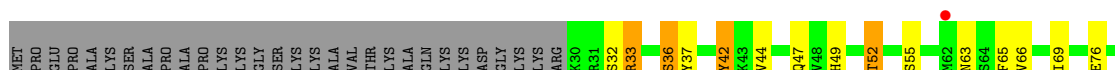
• Molecule 4: Histone H2B type 1-J



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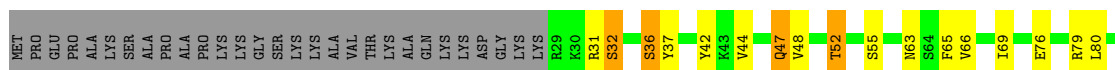


• Molecule 4: Histone H2B type 1-J

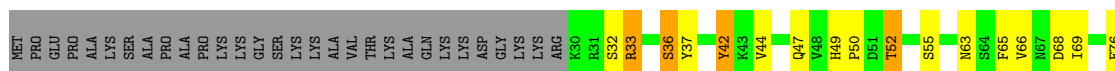




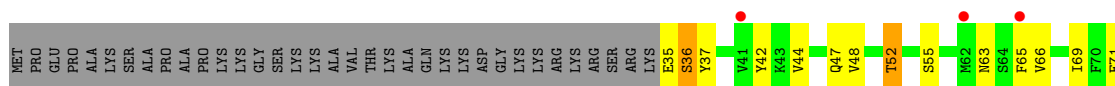
• Molecule 4: Histone H2B type 1-J



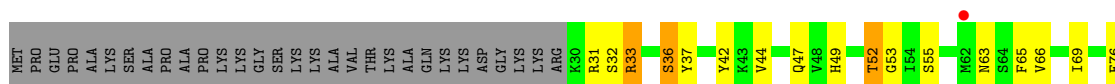
• Molecule 4: Histone H2B type 1-J



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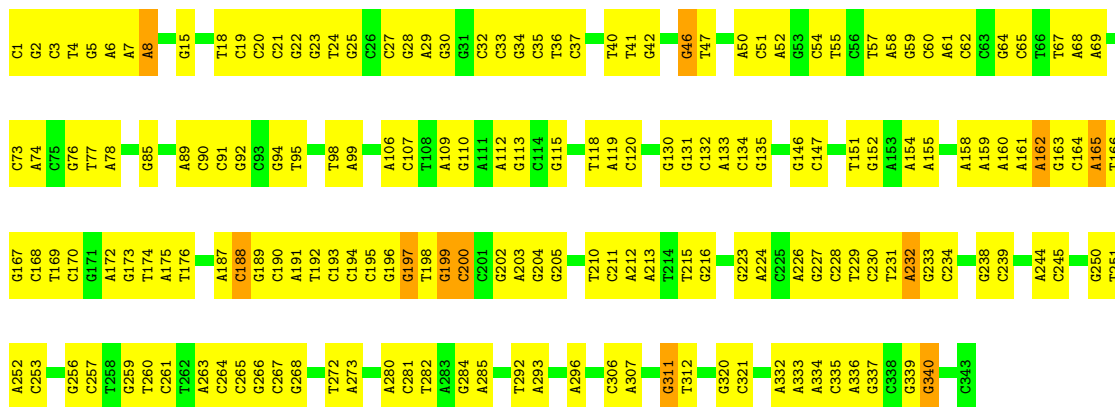


• Molecule 4: Histone H2B type 1-J

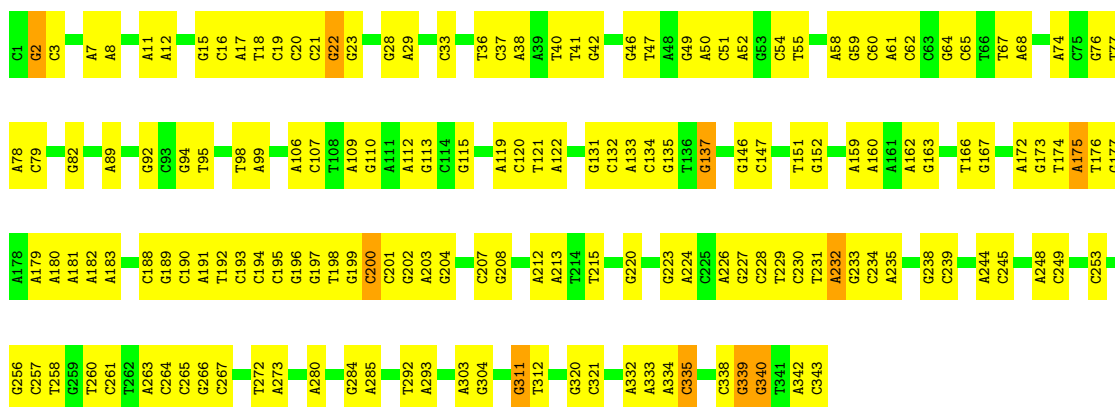


• Molecule 5: DNA (343-MER)





• Molecule 5: DNA (343-MER)

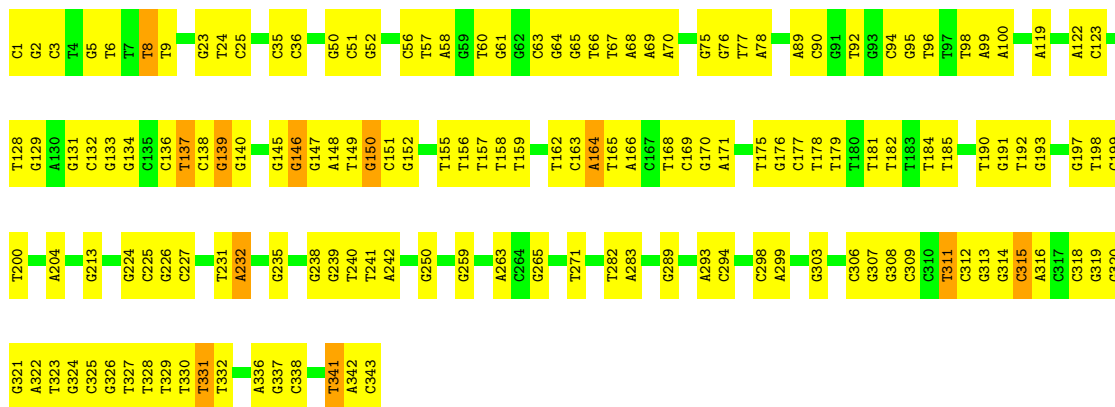


• Molecule 6: DNA (343-MER)

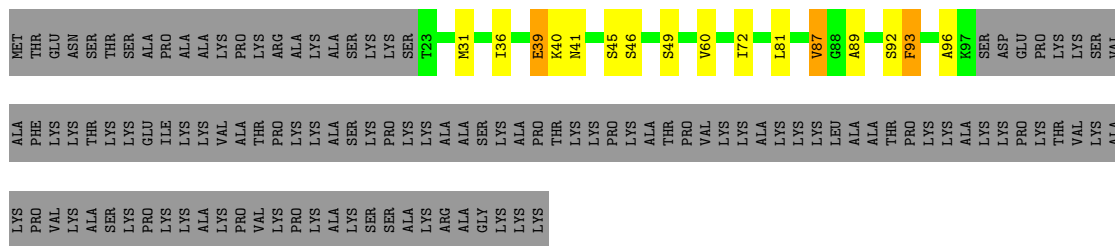


• Molecule 6: DNA (343-MER)

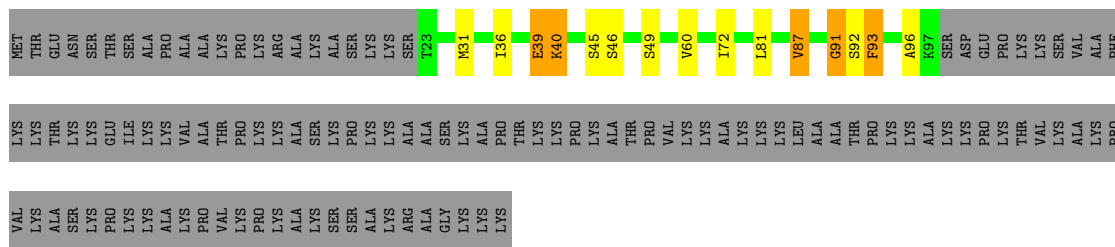




● Molecule 7: Histone H1.0



● Molecule 7: Histone H1.0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.75Å 205.90Å 237.68Å 90.00° 97.19° 90.00°	Depositor
Resolution (Å)	49.35 – 3.89 49.35 – 3.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.35-3.89) 99.3 (49.35-3.89)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.88Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.199 , 0.267 0.202 , 0.262	Depositor DCC
$R_{free}$ test set	1885 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	185.6	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 156.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	53828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	240.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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	1.02	0/837	1.48	0/1120
1	E	1.01	0/837	1.48	0/1120
1	K	1.00	0/828	1.48	0/1109
1	O	0.99	0/828	1.48	0/1109
1	U	1.00	0/828	1.47	0/1109
1	Y	1.00	0/837	1.48	0/1120
1	e	0.99	0/828	1.47	0/1109
1	i	1.01	0/837	1.48	0/1120
2	B	1.00	0/669	1.53	0/894
2	F	1.01	0/680	1.54	0/908
2	L	0.99	0/660	1.53	0/883
2	P	1.01	0/702	1.51	0/937
2	V	1.00	0/680	1.53	0/908
2	Z	0.99	0/691	1.53	0/923
2	f	0.99	0/660	1.53	0/883
2	j	1.00	0/653	1.54	0/873
3	C	1.04	0/854	1.55	0/1150
3	G	1.00	0/815	1.51	0/1100
3	M	1.02	0/854	1.54	0/1150
3	Q	1.00	0/829	1.54	0/1118
3	W	1.02	0/854	1.54	0/1150
3	a	1.01	0/806	1.52	0/1089
3	g	1.03	0/854	1.55	0/1150
3	k	1.01	0/845	1.51	0/1139
4	D	1.04	0/777	1.60	0/1040
4	H	1.02	0/766	1.59	0/1026
4	N	1.05	0/777	1.60	0/1040
4	R	1.04	0/766	1.59	0/1026
4	X	1.03	0/720	1.61	0/968
4	b	1.05	0/766	1.58	0/1026
4	h	1.09	0/766	1.67	4/1026 (0.4%)
4	l	1.04	0/766	1.58	0/1026
5	I	0.37	0/7890	0.82	14/12165 (0.1%)
5	c	0.36	0/7890	0.80	13/12165 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	J	0.37	0/7888	0.83	13/12180 (0.1%)
6	d	0.35	0/7888	0.81	15/12180 (0.1%)
7	S	1.15	0/581	1.45	0/775
7	T	1.15	0/581	1.46	1/775 (0.1%)
All	All	0.74	0/57588	1.17	60/83589 (0.1%)

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
2	P	0	1

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	h	31	ARG	NE-CZ-NH2	-10.27	109.95	119.20
5	I	162	DA	C2'-C3'-O3'	8.09	123.63	111.50
4	h	31	ARG	NE-CZ-NH1	7.76	129.26	121.50
5	I	200	DC	C2'-C3'-O3'	-7.44	100.34	111.50
6	d	150	DG	C4'-C3'-O3'	7.31	120.97	110.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	18	HIS	Peptide

## 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	825	0	869	19	0
1	E	825	0	869	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	816	0	856	16	1
1	O	816	0	856	8	0
1	U	816	0	856	13	0
1	Y	825	0	869	11	0
1	e	816	0	856	16	0
1	i	825	0	869	12	0
2	B	662	0	709	12	0
2	F	673	0	722	8	0
2	L	653	0	696	15	0
2	P	694	0	742	11	0
2	V	673	0	722	10	0
2	Z	683	0	729	23	0
2	f	653	0	696	4	0
2	j	646	0	687	12	1
3	C	844	0	910	16	0
3	G	805	0	861	12	1
3	M	844	0	910	14	0
3	Q	819	0	879	17	0
3	W	844	0	910	10	1
3	a	796	0	848	12	0
3	g	844	0	910	15	0
3	k	835	0	897	11	0
4	D	766	0	797	21	0
4	H	755	0	784	17	0
4	N	766	0	797	22	0
4	R	755	0	784	23	0
4	X	709	0	727	20	0
4	b	755	0	784	19	0
4	h	755	0	784	25	0
4	l	755	0	784	19	0
5	I	7024	0	3836	173	0
5	c	7024	0	3836	150	0
6	J	7041	0	3873	175	0
6	d	7041	0	3873	149	0
7	S	575	0	604	8	0
7	T	575	0	604	7	0
All	All	53828	0	42595	898	2

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 9.

The worst 5 of 898 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)
6:J:162:DT:H2''	6:J:163:DC:C5	1.81	1.15
6:J:175:DT:H1'	6:J:176:DG:O4'	1.42	1.15
6:J:113:DC:OP1	4:N:32:SER:OG	1.68	1.11
6:d:164:DA:H1'	6:d:165:DT:H5'	1.29	1.07
5:c:173:DG:H2''	5:c:174:DT:OP2	1.50	1.05

All (2) 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)
2:j:22:LEU:O	3:G:72:ASP:OD1[2_354]	2.09	0.11
1:K:77:ASP:OD1	3:W:64:GLU:OE2[2_555]	2.16	0.04

## 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	98/136 (72%)	83 (85%)	13 (13%)	2 (2%)	6	32
1	E	98/136 (72%)	84 (86%)	12 (12%)	2 (2%)	6	32
1	K	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)	5	31
1	O	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)	5	31
1	U	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)	5	31
1	Y	98/136 (72%)	84 (86%)	12 (12%)	2 (2%)	6	32
1	e	97/136 (71%)	82 (84%)	12 (12%)	3 (3%)	3	25
1	i	98/136 (72%)	83 (85%)	13 (13%)	2 (2%)	6	32
2	B	81/103 (79%)	62 (76%)	19 (24%)	0	100	100
2	F	82/103 (80%)	65 (79%)	17 (21%)	0	100	100
2	L	80/103 (78%)	64 (80%)	16 (20%)	0	100	100
2	P	84/103 (82%)	65 (77%)	18 (21%)	1 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	82/103 (80%)	64 (78%)	18 (22%)	0	100	100
2	Z	83/103 (81%)	64 (77%)	19 (23%)	0	100	100
2	f	80/103 (78%)	63 (79%)	17 (21%)	0	100	100
2	j	79/103 (77%)	61 (77%)	18 (23%)	0	100	100
3	C	107/130 (82%)	93 (87%)	13 (12%)	1 (1%)	14	47
3	G	102/130 (78%)	90 (88%)	11 (11%)	1 (1%)	12	45
3	M	107/130 (82%)	95 (89%)	11 (10%)	1 (1%)	14	47
3	Q	104/130 (80%)	92 (88%)	11 (11%)	1 (1%)	12	45
3	W	107/130 (82%)	94 (88%)	12 (11%)	1 (1%)	14	47
3	a	101/130 (78%)	89 (88%)	11 (11%)	1 (1%)	12	45
3	g	107/130 (82%)	94 (88%)	12 (11%)	1 (1%)	14	47
3	k	106/130 (82%)	93 (88%)	12 (11%)	1 (1%)	14	47
4	D	95/126 (75%)	73 (77%)	21 (22%)	1 (1%)	11	43
4	H	94/126 (75%)	71 (76%)	21 (22%)	2 (2%)	5	31
4	N	95/126 (75%)	73 (77%)	21 (22%)	1 (1%)	11	43
4	R	94/126 (75%)	71 (76%)	21 (22%)	2 (2%)	5	31
4	X	89/126 (71%)	70 (79%)	18 (20%)	1 (1%)	11	43
4	b	94/126 (75%)	70 (74%)	22 (23%)	2 (2%)	5	31
4	h	94/126 (75%)	72 (77%)	20 (21%)	2 (2%)	5	31
4	l	94/126 (75%)	70 (74%)	22 (23%)	2 (2%)	5	31
7	S	73/194 (38%)	59 (81%)	10 (14%)	4 (6%)	1	17
7	T	73/194 (38%)	59 (81%)	10 (14%)	4 (6%)	1	17
All	All	3167/4348 (73%)	2601 (82%)	519 (16%)	47 (2%)	8	37

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	l	33	ARG
4	H	33	ARG
7	S	87	VAL
7	T	87	VAL
2	P	18	HIS

### 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	87/111 (78%)	85 (98%)	2 (2%)	44	63
1	E	87/111 (78%)	84 (97%)	3 (3%)	32	55
1	K	86/111 (78%)	84 (98%)	2 (2%)	44	63
1	O	86/111 (78%)	83 (96%)	3 (4%)	32	54
1	U	86/111 (78%)	84 (98%)	2 (2%)	44	63
1	Y	87/111 (78%)	84 (97%)	3 (3%)	32	55
1	e	86/111 (78%)	84 (98%)	2 (2%)	44	63
1	i	87/111 (78%)	83 (95%)	4 (5%)	24	48
2	B	68/79 (86%)	64 (94%)	4 (6%)	18	44
2	F	69/79 (87%)	66 (96%)	3 (4%)	26	49
2	L	67/79 (85%)	63 (94%)	4 (6%)	17	44
2	P	71/79 (90%)	67 (94%)	4 (6%)	19	45
2	V	69/79 (87%)	65 (94%)	4 (6%)	18	44
2	Z	70/79 (89%)	66 (94%)	4 (6%)	18	44
2	f	67/79 (85%)	63 (94%)	4 (6%)	17	44
2	j	66/79 (84%)	63 (96%)	3 (4%)	24	49
3	C	86/100 (86%)	81 (94%)	5 (6%)	18	44
3	G	83/100 (83%)	77 (93%)	6 (7%)	13	39
3	M	86/100 (86%)	82 (95%)	4 (5%)	23	48
3	Q	84/100 (84%)	76 (90%)	8 (10%)	8	29
3	W	86/100 (86%)	82 (95%)	4 (5%)	23	48
3	a	82/100 (82%)	77 (94%)	5 (6%)	17	43
3	g	86/100 (86%)	82 (95%)	4 (5%)	23	48
3	k	85/100 (85%)	79 (93%)	6 (7%)	13	40
4	D	83/105 (79%)	72 (87%)	11 (13%)	4	19
4	H	82/105 (78%)	72 (88%)	10 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	83/105 (79%)	71 (86%)	12 (14%)	3	17
4	R	82/105 (78%)	69 (84%)	13 (16%)	2	14
4	X	77/105 (73%)	67 (87%)	10 (13%)	4	19
4	b	82/105 (78%)	70 (85%)	12 (15%)	3	16
4	h	82/105 (78%)	71 (87%)	11 (13%)	4	19
4	l	82/105 (78%)	69 (84%)	13 (16%)	2	14
7	S	62/158 (39%)	54 (87%)	8 (13%)	4	20
7	T	62/158 (39%)	54 (87%)	8 (13%)	4	20
All	All	2694/3476 (78%)	2493 (92%)	201 (8%)	12	38

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	74	LYS
3	Q	119	LYS
4	b	123	SER
4	N	36	SER
1	O	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	108	ASN
3	W	24	GLN
2	P	64	ASN
4	R	47	GLN
3	W	68	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 oligosaccharides 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 i

### 6.1 Protein, DNA and RNA chains i

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	100/136 (73%)	-0.78	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	122, 175, 243, 313	0
1	E	100/136 (73%)	-0.58	1 (1%) <span style="border: 1px solid blue; padding: 2px;">79</span> <span style="border: 1px solid blue; padding: 2px;">59</span>	89, 163, 240, 277	0
1	K	99/136 (72%)	-0.65	1 (1%) <span style="border: 1px solid blue; padding: 2px;">79</span> <span style="border: 1px solid blue; padding: 2px;">59</span>	125, 168, 232, 344	0
1	O	99/136 (72%)	-0.51	4 (4%) <span style="border: 1px solid red; padding: 2px;">42</span> <span style="border: 1px solid red; padding: 2px;">31</span>	133, 192, 258, 309	0
1	U	99/136 (72%)	-0.59	2 (2%) <span style="border: 1px solid blue; padding: 2px;">65</span> <span style="border: 1px solid blue; padding: 2px;">45</span>	112, 166, 226, 290	0
1	Y	100/136 (73%)	-0.61	2 (2%) <span style="border: 1px solid blue; padding: 2px;">65</span> <span style="border: 1px solid blue; padding: 2px;">45</span>	146, 211, 270, 310	0
1	e	99/136 (72%)	-0.46	5 (5%) <span style="border: 1px solid red; padding: 2px;">33</span> <span style="border: 1px solid red; padding: 2px;">26</span>	122, 191, 265, 313	0
1	i	100/136 (73%)	-0.68	1 (1%) <span style="border: 1px solid blue; padding: 2px;">79</span> <span style="border: 1px solid blue; padding: 2px;">59</span>	123, 173, 259, 297	0
2	B	83/103 (80%)	-0.68	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	112, 162, 226, 452	0
2	F	84/103 (81%)	-0.55	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	112, 162, 280, 391	0
2	L	82/103 (79%)	-0.48	2 (2%) <span style="border: 1px solid blue; padding: 2px;">59</span> <span style="border: 1px solid red; padding: 2px;">42</span>	125, 161, 208, 255	0
2	P	86/103 (83%)	-0.42	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	140, 202, 306, 364	0
2	V	84/103 (81%)	-0.64	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	118, 159, 249, 399	0
2	Z	85/103 (82%)	-0.53	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	143, 204, 283, 336	0
2	f	82/103 (79%)	-0.51	1 (1%) <span style="border: 1px solid blue; padding: 2px;">76</span> <span style="border: 1px solid blue; padding: 2px;">55</span>	144, 190, 231, 423	0
2	j	81/103 (78%)	-0.59	1 (1%) <span style="border: 1px solid blue; padding: 2px;">76</span> <span style="border: 1px solid blue; padding: 2px;">55</span>	116, 162, 219, 338	0
3	C	109/130 (83%)	-0.61	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	103, 167, 239, 270	0
3	G	104/130 (80%)	-0.60	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	128, 183, 243, 285	0
3	M	109/130 (83%)	-0.69	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	162, 220, 297, 357	0
3	Q	106/130 (81%)	-0.65	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	125, 196, 262, 323	0
3	W	109/130 (83%)	-0.35	3 (2%) <span style="border: 1px solid blue; padding: 2px;">55</span> <span style="border: 1px solid red; padding: 2px;">38</span>	116, 185, 264, 298	0
3	a	103/130 (79%)	-0.62	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	126, 197, 273, 365	0
3	g	109/130 (83%)	-0.74	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	109, 175, 267, 308	0
3	k	108/130 (83%)	-0.57	2 (1%) <span style="border: 1px solid blue; padding: 2px;">66</span> <span style="border: 1px solid red; padding: 2px;">46</span>	163, 213, 278, 360	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
4	D	97/126 (76%)	-0.73	0 100 100	110, 169, 252, 326	0
4	H	96/126 (76%)	-0.70	1 (1%) 79 59	109, 180, 245, 282	0
4	N	97/126 (76%)	-0.65	1 (1%) 79 59	155, 220, 301, 328	0
4	R	96/126 (76%)	-0.69	1 (1%) 79 59	145, 201, 264, 298	0
4	X	91/126 (72%)	-0.51	3 (3%) 49 34	125, 178, 240, 296	0
4	b	96/126 (76%)	-0.58	1 (1%) 79 59	127, 209, 267, 330	0
4	h	96/126 (76%)	-0.81	0 100 100	122, 181, 250, 298	0
4	l	96/126 (76%)	-0.60	1 (1%) 79 59	154, 213, 286, 318	0
5	I	343/343 (100%)	-0.78	0 100 100	151, 264, 394, 469	0
5	c	343/343 (100%)	-0.80	0 100 100	155, 266, 391, 518	0
6	J	343/343 (100%)	-0.76	0 100 100	112, 266, 386, 446	0
6	d	343/343 (100%)	-0.78	0 100 100	159, 274, 404, 479	0
7	S	75/194 (38%)	-0.78	0 100 100	234, 312, 398, 432	1 (1%)
7	T	75/194 (38%)	-0.80	0 100 100	258, 348, 409, 437	1 (1%)
All	All	4607/5720 (80%)	-0.67	33 (0%) 84 67	89, 209, 350, 518	2 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	X	62	MET	3.8
1	e	67	PHE	3.7
1	O	96	CYS	3.5
3	W	62	ILE	3.4
1	Y	56	LYS	3.4

## 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 oligosaccharides 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.