



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 19, 2026 – 09:41 PM UTC

PDB ID : 6HKT / pdb_00006hkt
Title : Structure of an H1-bound 6-nucleosome array
Authors : Garcia-Saez, I.; Dimitrov, S.; Petosa, C.
Deposited on : 2018-09-08
Resolution : 9.70 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

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>.

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

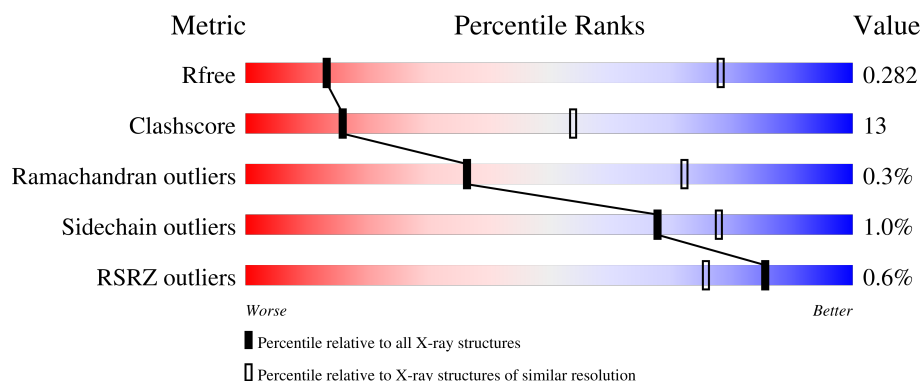
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.70 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	1168 (11.50-4.00)
Clashscore	190562	1002 (15.00-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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 ≥ 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	139	
1	E	139	
1	K	139	
1	O	139	
1	U	139	

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Mol	Chain	Length	Quality of chain
1	Y	139	
1	a	139	
1	e	139	
1	k	139	
1	o	139	
1	u	139	
1	y	139	
2	B	106	
2	F	106	
2	L	106	
2	P	106	
2	V	106	
2	Z	106	
2	b	106	
2	f	106	
2	l	106	
2	p	106	
2	v	106	
2	z	106	
3	0	133	
3	2	133	
3	C	133	
3	G	133	
3	M	133	
3	Q	133	

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Mol	Chain	Length	Quality of chain
3	W	133	
3	c	133	
3	g	133	
3	m	133	
3	q	133	
3	w	133	
4	1	129	
4	3	129	
4	D	129	
4	H	129	
4	N	129	
4	R	129	
4	X	129	
4	d	129	
4	h	129	
4	n	129	
4	r	129	
4	x	129	
5	I	1122	
6	J	1122	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 82122 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
1	A	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	E	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	a	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	e	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	K	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	O	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	k	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	o	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	U	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	Y	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	u	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	y	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	HIS	-	expression tag	UNP P68431
a	-3	GLY	-	expression tag	UNP P68431
a	-2	SER	-	expression tag	UNP P68431
a	-1	HIS	-	expression tag	UNP P68431
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431
K	-3	GLY	-	expression tag	UNP P68431
K	-2	SER	-	expression tag	UNP P68431
K	-1	HIS	-	expression tag	UNP P68431
O	-3	GLY	-	expression tag	UNP P68431
O	-2	SER	-	expression tag	UNP P68431
O	-1	HIS	-	expression tag	UNP P68431
k	-3	GLY	-	expression tag	UNP P68431
k	-2	SER	-	expression tag	UNP P68431
k	-1	HIS	-	expression tag	UNP P68431
o	-3	GLY	-	expression tag	UNP P68431
o	-2	SER	-	expression tag	UNP P68431
o	-1	HIS	-	expression tag	UNP P68431
U	-3	GLY	-	expression tag	UNP P68431
U	-2	SER	-	expression tag	UNP P68431
U	-1	HIS	-	expression tag	UNP P68431
Y	-3	GLY	-	expression tag	UNP P68431
Y	-2	SER	-	expression tag	UNP P68431
Y	-1	HIS	-	expression tag	UNP P68431
u	-3	GLY	-	expression tag	UNP P68431
u	-2	SER	-	expression tag	UNP P68431
u	-1	HIS	-	expression tag	UNP P68431
y	-3	GLY	-	expression tag	UNP P68431
y	-2	SER	-	expression tag	UNP P68431
y	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	F	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	b	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	f	82	Total 653	C 412	N 127	O 113	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	P	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	l	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	p	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	V	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	Z	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	v	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	z	82	Total 653	C 412	N 127	O 113	S 1	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
L	-3	GLY	-	expression tag	UNP P62805
L	-2	SER	-	expression tag	UNP P62805
L	-1	HIS	-	expression tag	UNP P62805
P	-3	GLY	-	expression tag	UNP P62805
P	-2	SER	-	expression tag	UNP P62805
P	-1	HIS	-	expression tag	UNP P62805
l	-3	GLY	-	expression tag	UNP P62805
l	-2	SER	-	expression tag	UNP P62805
l	-1	HIS	-	expression tag	UNP P62805
p	-3	GLY	-	expression tag	UNP P62805
p	-2	SER	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
p	-1	HIS	-	expression tag	UNP P62805
V	-3	GLY	-	expression tag	UNP P62805
V	-2	SER	-	expression tag	UNP P62805
V	-1	HIS	-	expression tag	UNP P62805
Z	-3	GLY	-	expression tag	UNP P62805
Z	-2	SER	-	expression tag	UNP P62805
Z	-1	HIS	-	expression tag	UNP P62805
v	-3	GLY	-	expression tag	UNP P62805
v	-2	SER	-	expression tag	UNP P62805
v	-1	HIS	-	expression tag	UNP P62805
z	-3	GLY	-	expression tag	UNP P62805
z	-2	SER	-	expression tag	UNP P62805
z	-1	HIS	-	expression tag	UNP P62805

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	G	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	c	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	g	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	M	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	Q	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	m	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	q	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	W	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	0	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	w	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	2	103	Total	C	N	O	0	0	0
			796	502	155	139			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908
M	-3	GLY	-	expression tag	UNP P04908
M	-2	SER	-	expression tag	UNP P04908
M	-1	HIS	-	expression tag	UNP P04908
Q	-3	GLY	-	expression tag	UNP P04908
Q	-2	SER	-	expression tag	UNP P04908
Q	-1	HIS	-	expression tag	UNP P04908
m	-3	GLY	-	expression tag	UNP P04908
m	-2	SER	-	expression tag	UNP P04908
m	-1	HIS	-	expression tag	UNP P04908
q	-3	GLY	-	expression tag	UNP P04908
q	-2	SER	-	expression tag	UNP P04908
q	-1	HIS	-	expression tag	UNP P04908
W	-3	GLY	-	expression tag	UNP P04908
W	-2	SER	-	expression tag	UNP P04908
W	-1	HIS	-	expression tag	UNP P04908
0	-3	GLY	-	expression tag	UNP P04908
0	-2	SER	-	expression tag	UNP P04908
0	-1	HIS	-	expression tag	UNP P04908
w	-3	GLY	-	expression tag	UNP P04908
w	-2	SER	-	expression tag	UNP P04908
w	-1	HIS	-	expression tag	UNP P04908
2	-3	GLY	-	expression tag	UNP P04908
2	-2	SER	-	expression tag	UNP P04908
2	-1	HIS	-	expression tag	UNP P04908

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	H	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	h	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	N	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	R	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	n	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	r	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	X	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	1	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	x	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	3	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP P06899
D	-5	SER	-	expression tag	UNP P06899
D	-4	HIS	-	expression tag	UNP P06899
H	-6	GLY	-	expression tag	UNP P06899
H	-5	SER	-	expression tag	UNP P06899
H	-4	HIS	-	expression tag	UNP P06899
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899
N	-6	GLY	-	expression tag	UNP P06899
N	-5	SER	-	expression tag	UNP P06899
N	-4	HIS	-	expression tag	UNP P06899
R	-6	GLY	-	expression tag	UNP P06899
R	-5	SER	-	expression tag	UNP P06899
R	-4	HIS	-	expression tag	UNP P06899
n	-6	GLY	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
n	-5	SER	-	expression tag	UNP P06899
n	-4	HIS	-	expression tag	UNP P06899
r	-6	GLY	-	expression tag	UNP P06899
r	-5	SER	-	expression tag	UNP P06899
r	-4	HIS	-	expression tag	UNP P06899
X	-6	GLY	-	expression tag	UNP P06899
X	-5	SER	-	expression tag	UNP P06899
X	-4	HIS	-	expression tag	UNP P06899
1	-6	GLY	-	expression tag	UNP P06899
1	-5	SER	-	expression tag	UNP P06899
1	-4	HIS	-	expression tag	UNP P06899
x	-6	GLY	-	expression tag	UNP P06899
x	-5	SER	-	expression tag	UNP P06899
x	-4	HIS	-	expression tag	UNP P06899
3	-6	GLY	-	expression tag	UNP P06899
3	-5	SER	-	expression tag	UNP P06899
3	-4	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (1122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	1122	Total	C	N	O	P	0	0	0
			22861	10850	4162	6727	1122			

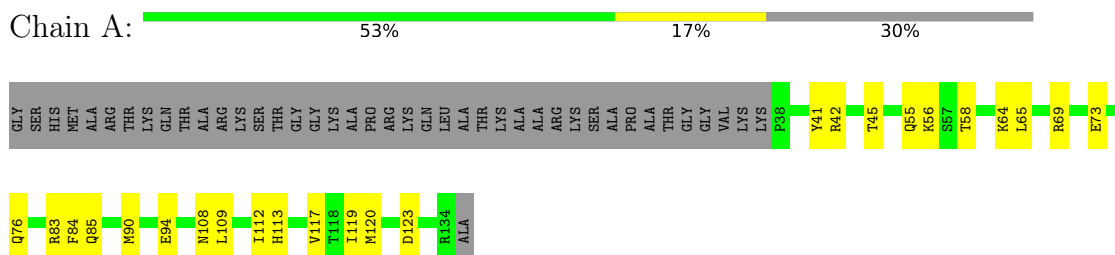
- Molecule 6 is a DNA chain called DNA (1122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	1122	Total	C	N	O	P	0	0	0
			23141	10945	4337	6737	1122			

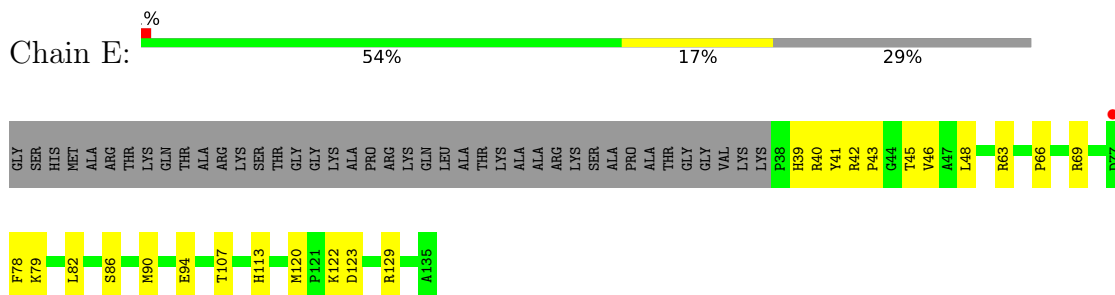
3 Residue-property plots [i](#)

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.

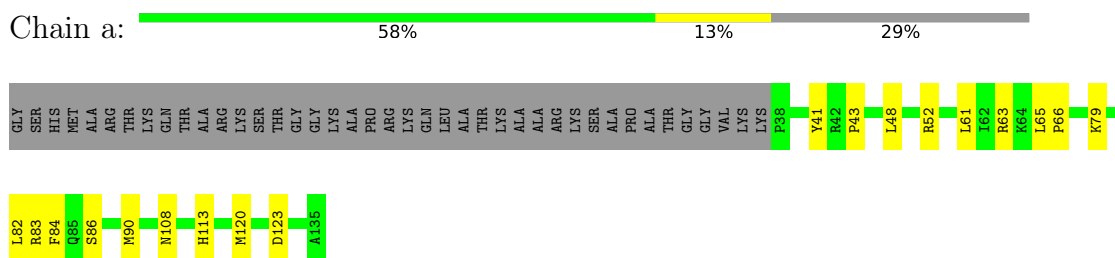
• Molecule 1: Histone H3.1



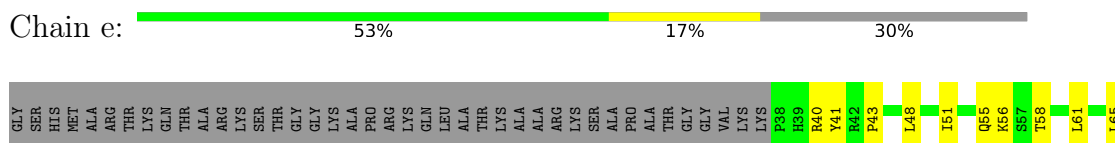
• Molecule 1: Histone H3.1



• Molecule 1: Histone H3.1

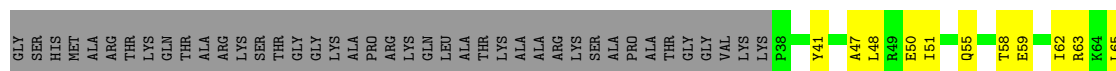


• Molecule 1: Histone H3.1

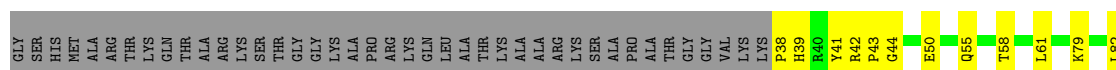




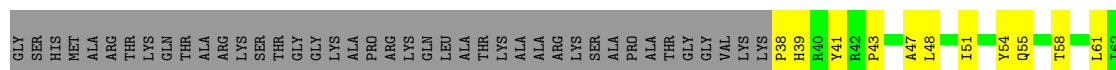
• Molecule 1: Histone H3.1



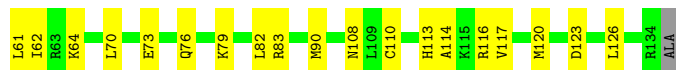
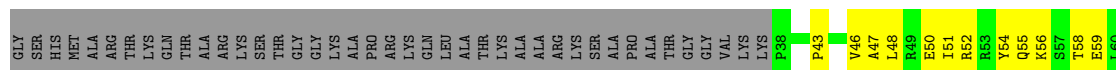
• Molecule 1: Histone H3.1



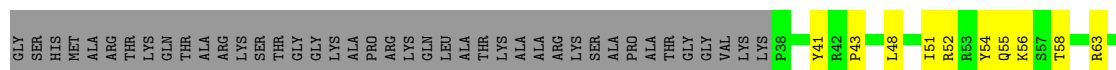
• Molecule 1: Histone H3.1



• Molecule 1: Histone H3.1



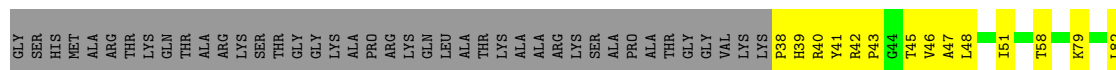
• Molecule 1: Histone H3.1





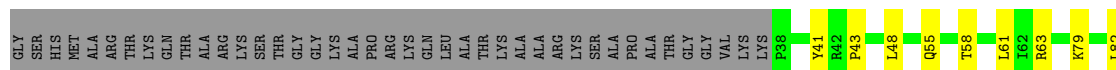
- Molecule 1: Histone H3.1

Chain Y: 48% 22% 29%



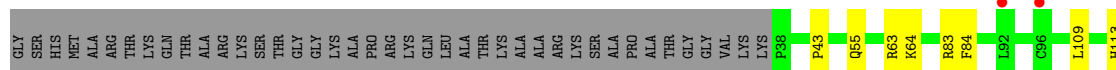
- Molecule 1: Histone H3.1

Chain u: 55% 15% 29%



- Molecule 1: Histone H3.1

Chain y: 64% 6% 30%



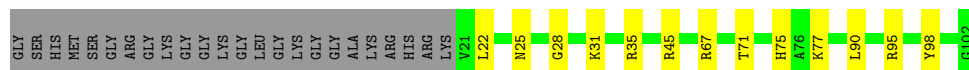
- Molecule 2: Histone H4

Chain B: 60% 17% 23%



- Molecule 2: Histone H4

Chain F: 65% 12% 23%



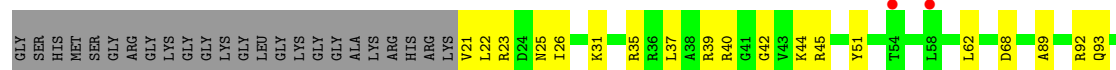
- Molecule 2: Histone H4



• Molecule 2: Histone H4



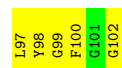
• Molecule 2: Histone H4



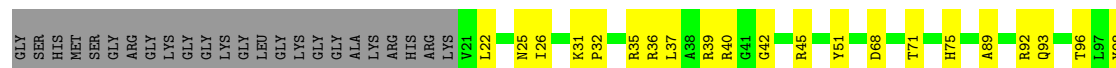
• Molecule 2: Histone H4



• Molecule 2: Histone H4



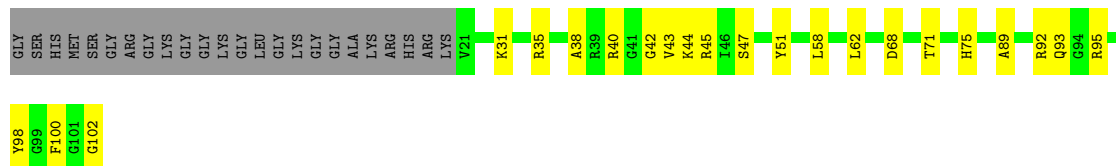
• Molecule 2: Histone H4





- Molecule 2: Histone H4

Chain V: 57% 21% 23%



- Molecule 2: Histone H4

Chain Z: 56% 22% 23%



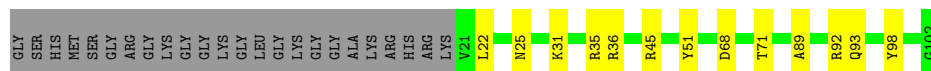
- Molecule 2: Histone H4

Chain v: 68% 9% 23%



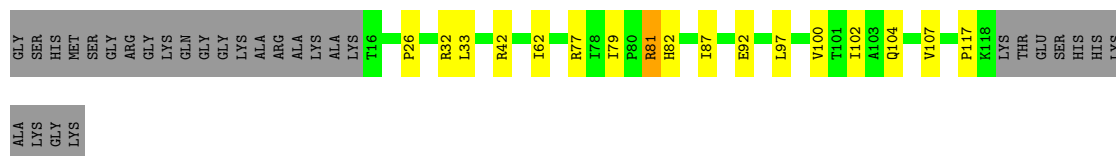
- Molecule 2: Histone H4

Chain z: 65% 12% 23%



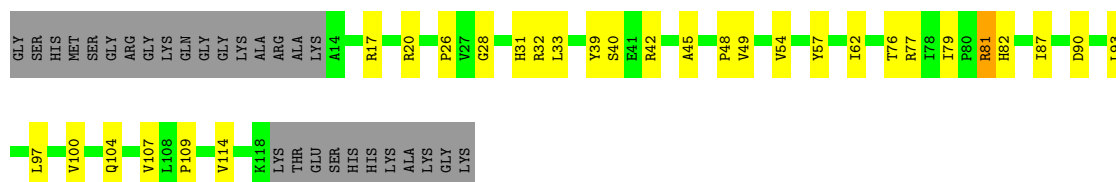
- Molecule 3: Histone H2A type 1-B/E

Chain C: 65% 12% 23%

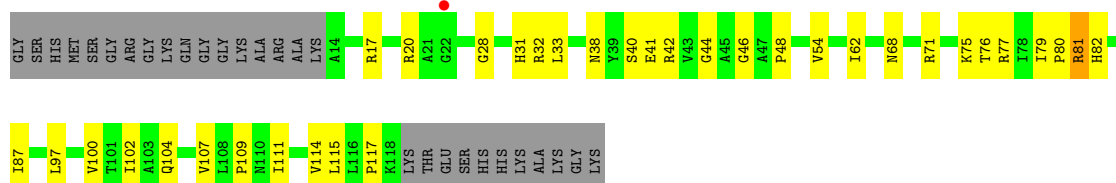


- Molecule 3: Histone H2A type 1-B/E

Chain G: 56% 22% 21%



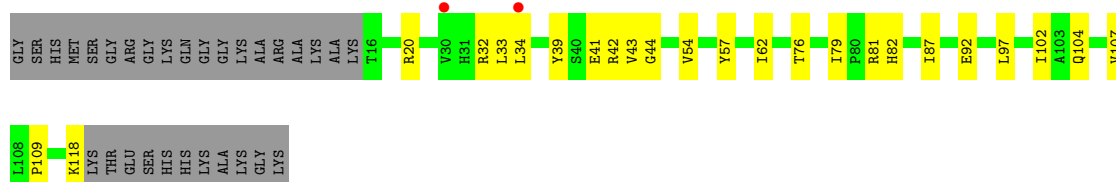
- Molecule 3: Histone H2A type 1-B/E



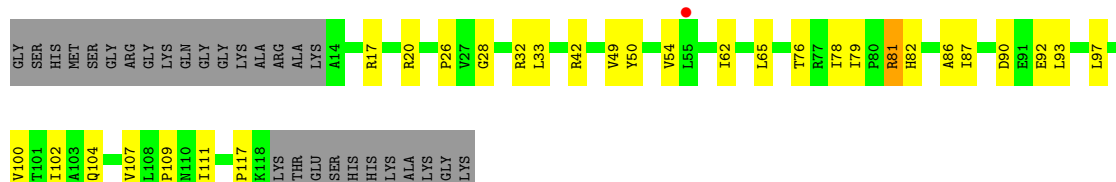
- Molecule 3: Histone H2A type 1-B/E



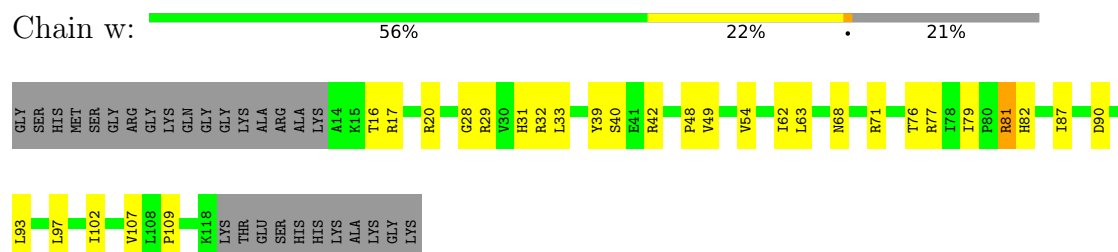
- Molecule 3: Histone H2A type 1-B/E



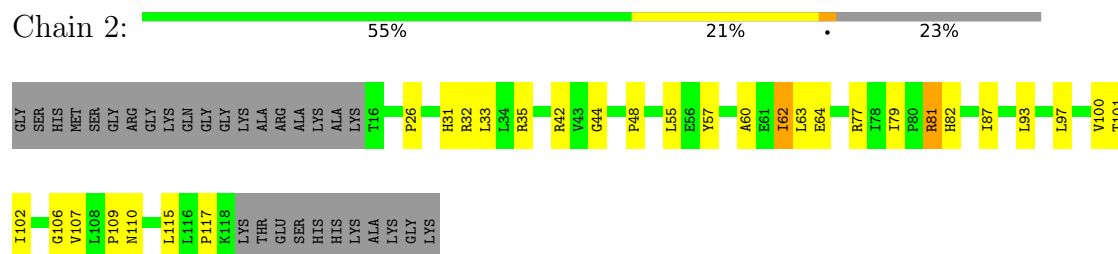
- Molecule 3: Histone H2A type 1-B/E



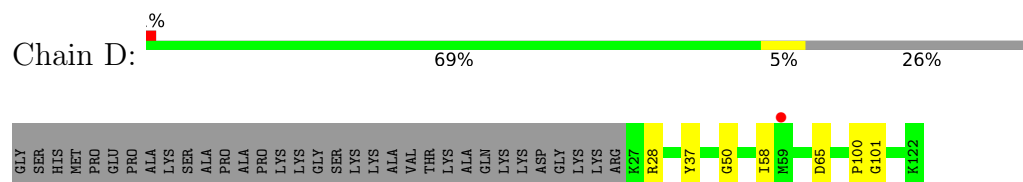
- Molecule 3: Histone H2A type 1-B/E



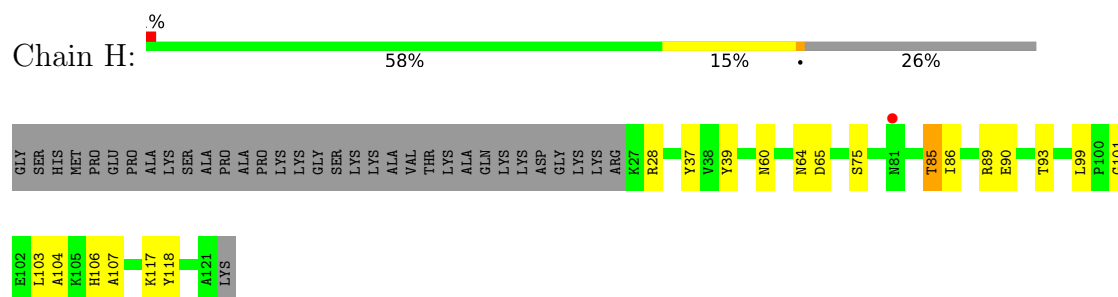
- Molecule 3: Histone H2A type 1-B/E



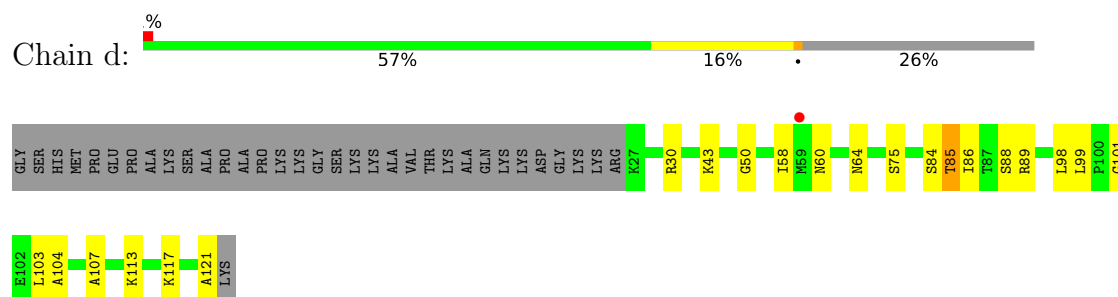
- Molecule 4: Histone H2B type 1-J



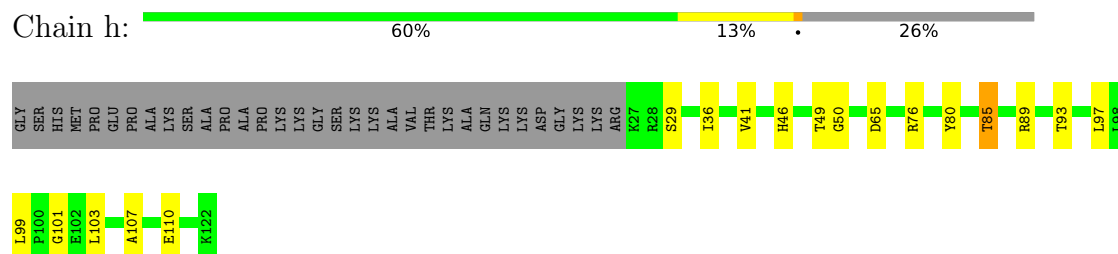
- Molecule 4: Histone H2B type 1-J



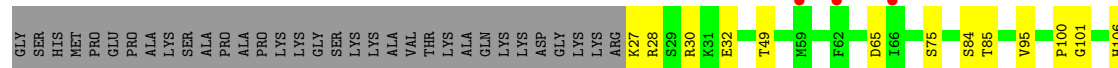
- Molecule 4: Histone H2B type 1-J



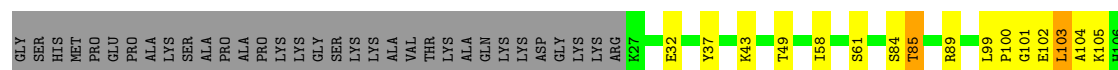
- Molecule 4: Histone H2B type 1-J



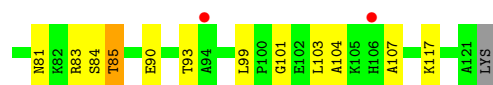
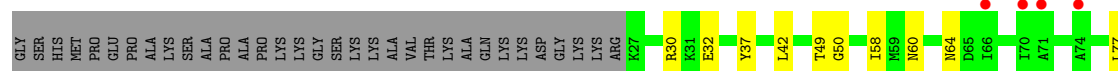
- Molecule 4: Histone H2B type 1-J



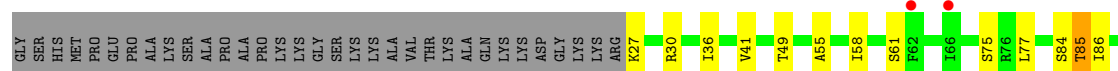
- Molecule 4: Histone H2B type 1-J



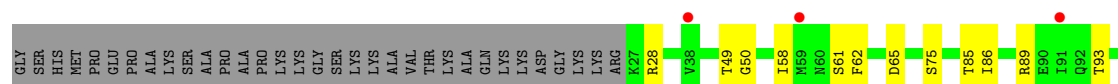
- Molecule 4: Histone H2B type 1-J



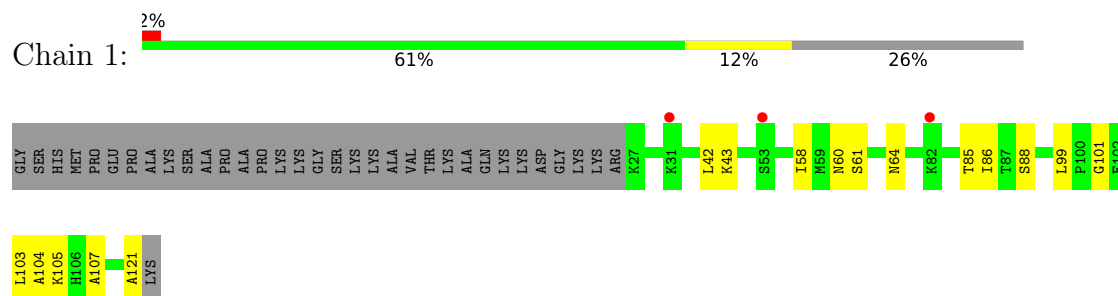
- Molecule 4: Histone H2B type 1-J



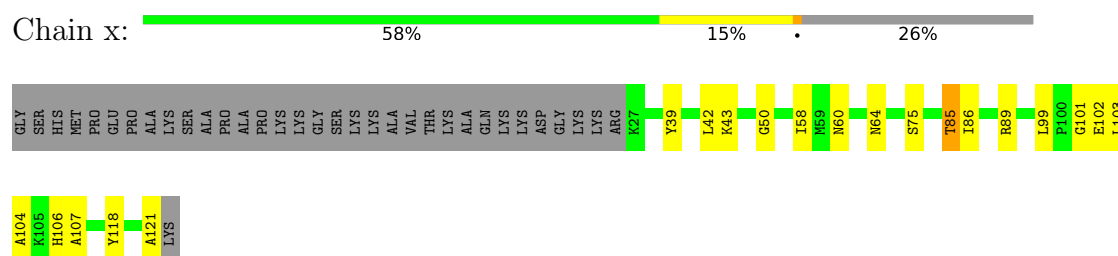
- Molecule 4: Histone H2B type 1-J



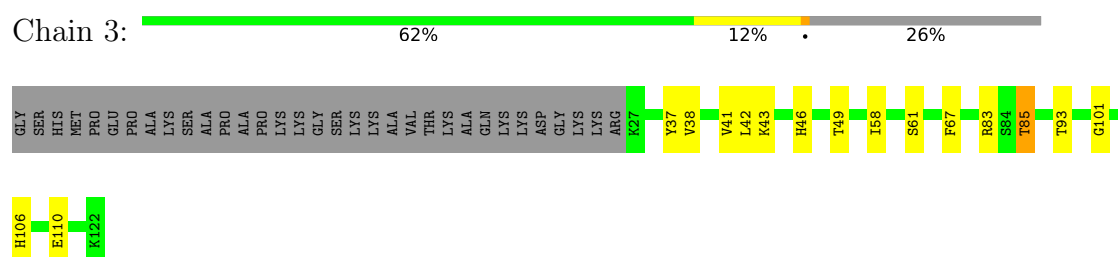
- Molecule 4: Histone H2B type 1-J



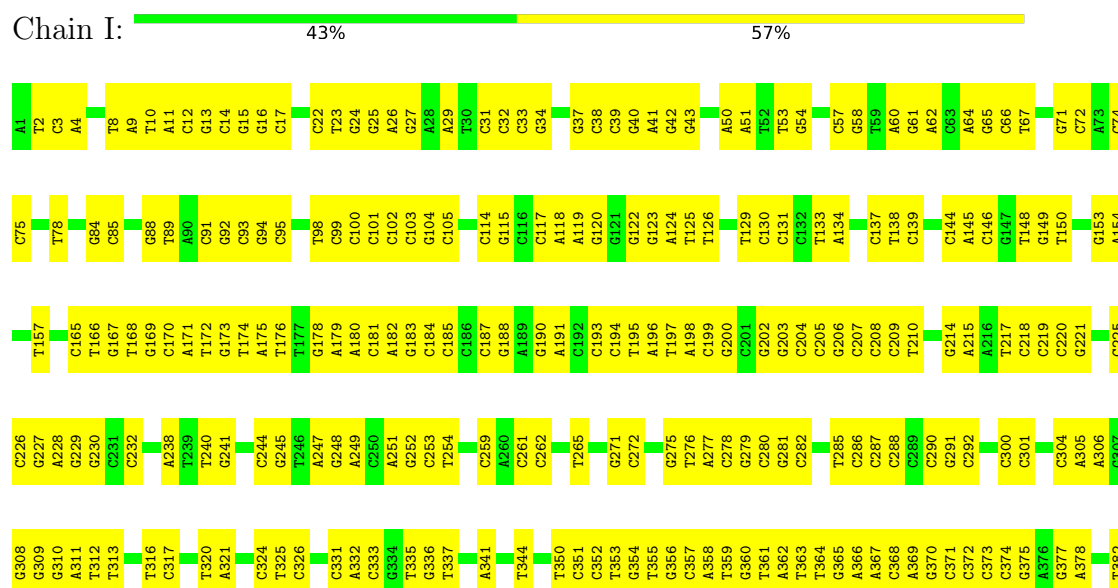
- Molecule 4: Histone H2B type 1-J

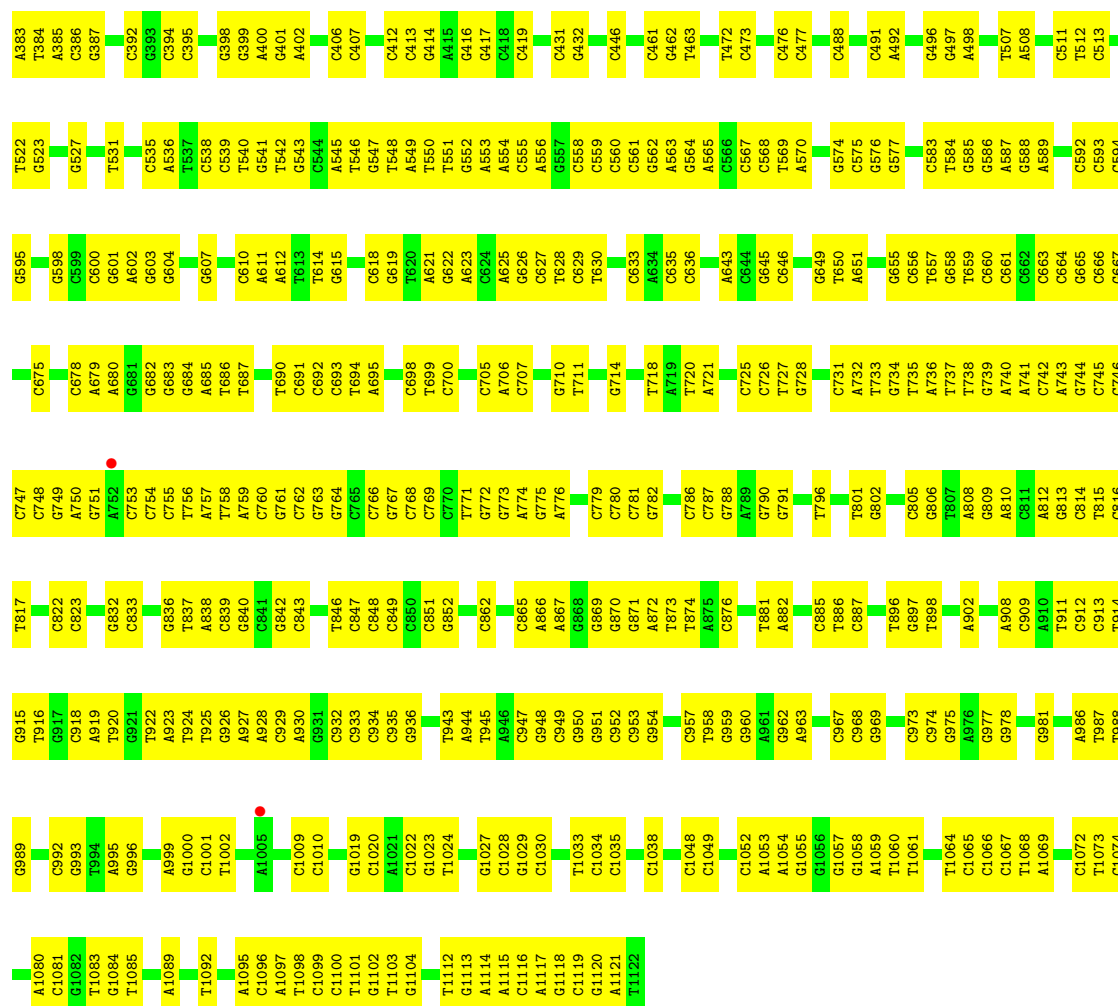


- Molecule 4: Histone H2B type 1-J



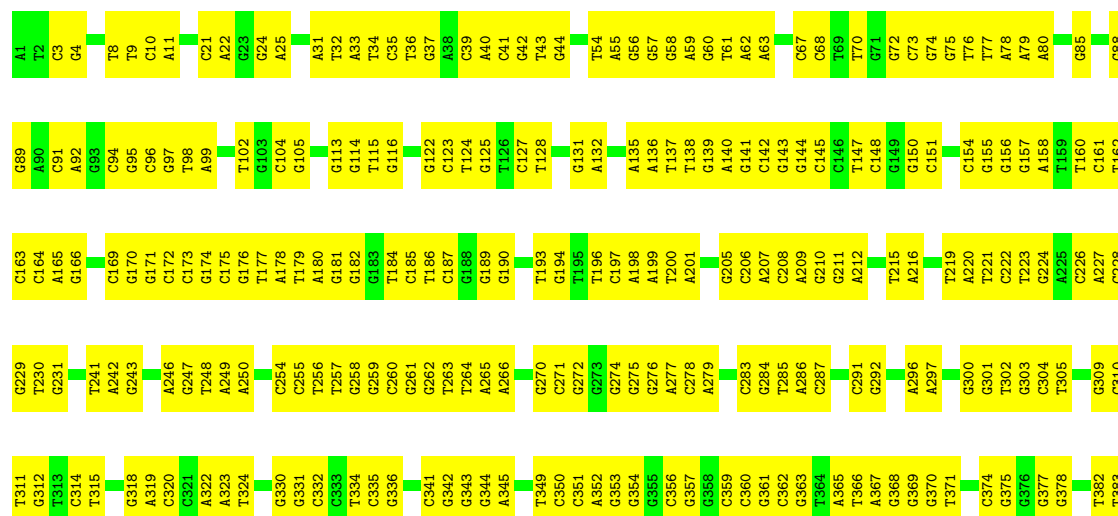
- Molecule 5: DNA (1122-MER)





• Molecule 6: DNA (1122-MER)

Chain J: 38% 62%



C384	G460	A532	C709	T784	T863	G938	G1010	
A385	G461	A620	G710	G785	G864	G939	T1011	C1086
A386	G462	G621				C940	T1012	
T387	G463		C715	A788	G870	T941	A1013	C1089
A388	A464	C627	G716	C789	C871	G942	A1014	G1090
C389	C465	C628	G717	G790		T943		G1091
A390	A466	A639	G718	T791	C875	T944	C1019	G1092
T391	G467	T631	G719	G792	T876	C945	G1020	A1093
	C468		T720			A946	G1021	T1094
A394	C469	G635	T721	A798	G879	A947	G1022	C1096
C395	C470	C543	T722		A880	T948	G1023	
	G471		T723	T802	C881	C949	G1024	C1099
A403	T472	G550	T724	A803	C882	C950	A1025	A1100
T404	A473	T551		G804	A883	A951	C1026	G1101
A406	G474	A552	C730	G805	A884	T952	A1027	G1102
T407	C475	T553	G731	G806	T885	G953	G1028	G1103
A408		A554	G732	A807		C954	C1029	C1104
C409	C478	G555		G808	C890	A955	G1030	G1105
T410	G479	G556	G737	T809	G891		C1031	C1106
G411	A484	T598	T738	A810	G892	G958	G1032	C1107
A412		G563	A739	A811	C893	G959	T1033	C1108
A414	G487	G564	T740		C894	A960	A1034	G1109
C415	T488		A741	C814	T895			
G416	G489		G742	C815	C896		C1039	T1122
T417	G490		G743	C816	G897	T965	G1040	
			G744	T817	G898	A966		
G422			T745	T818	C899	T967	A1045	
C423	C497		G746	G819	A900	A968	G1046	
A424	T498		T747	C820	C901	T969	G1047	
	G499		C748	C821	C902	C970	G1048	
T500	T500		G749	G822	G903	T971	G1049	
C501			G750	G823	G904	G972	T1050	
T502			G751	T824	G905		G1051	
	A506		G752	T825	A906	A975		
G505			C753	A826		C976	G1055	
A506			T754	A827	C909	T977	A1056	
			G755		T910	G978	G1057	
A509			T756	C832	C911	G979	C1058	
A510			C673	G833	C912		T1059	
T511			G674	G834		G984	G1060	
C512			G675	G835	G918			
G513			T676	G836	G919	T989	T1061	
				G837	C920	A990	C1062	
C440			A680	A838	C921	G991	T1063	
C441			G683	C839	G922	G992	G1066	
G446			C684	A840	C923	G993	A1067	
C447			T593	G841	G924	A994		
G448			A594	C842	T925	G995	A1070	
C449			T689	G843	A926	T996	T1071	
T450				A768	T927	A997	T1072	
T451			G892	G844	A928	A998	T1073	
A452			A693	G845	G929		G1074	
A453			G772	T846	G930	C1002		
C525			A773	A847	C848	C1003	G1078	
			T698			T1004	T1079	
C528				A858		C933	C1080	
G529			G704	G859		T934	C1081	
G530			G705	C860		G935	T1082	
			T708	G861		G936		
				G862		G937	C1083	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	111.08Å 238.76Å 674.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 9.70 49.07 – 9.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.07-9.70) 98.8 (49.07-9.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 9.80Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.254 , 0.286 0.256 , 0.282	Depositor DCC
R_{free} test set	573 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	339.6	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 306.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	82122	wwPDB-VP
Average B, all atoms (Å ²)	544.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.14	0/813	0.34	0/1090
1	E	0.12	0/819	0.33	0/1097
1	K	0.16	0/813	0.38	0/1090
1	O	0.13	0/819	0.34	0/1097
1	U	0.13	0/813	0.34	0/1090
1	Y	0.13	0/819	0.35	0/1097
1	a	0.12	0/819	0.33	0/1097
1	e	0.17	0/813	0.36	0/1090
1	k	0.16	0/819	0.39	0/1097
1	o	0.13	0/813	0.36	0/1090
1	u	0.15	0/819	0.36	0/1097
1	y	0.14	0/813	0.34	0/1090
2	B	0.18	0/660	0.38	0/883
2	F	0.18	0/660	0.39	0/883
2	L	0.17	0/660	0.37	0/883
2	P	0.18	0/660	0.38	0/883
2	V	0.21	0/660	0.42	0/883
2	Z	0.19	0/660	0.42	0/883
2	b	0.20	0/660	0.39	0/883
2	f	0.21	0/660	0.40	0/883
2	l	0.31	0/660	0.56	1/883 (0.1%)
2	p	0.24	0/660	0.43	0/883
2	v	0.19	0/660	0.41	0/883
2	z	0.19	0/660	0.37	0/883
3	0	0.14	0/820	0.35	0/1107
3	2	0.13	0/806	0.35	0/1089
3	C	0.13	0/806	0.32	0/1089
3	G	0.20	0/820	0.33	0/1107
3	M	0.11	0/806	0.32	0/1089
3	Q	0.12	0/820	0.33	0/1107
3	W	0.11	0/806	0.33	0/1089
3	c	0.18	0/820	0.38	0/1107
3	g	0.11	0/806	0.32	0/1089
3	m	0.15	0/820	0.35	0/1107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	q	0.15	0/806	0.37	0/1089
3	w	0.16	0/820	0.35	0/1107
4	1	0.14	0/756	0.33	0/1015
4	3	0.28	0/766	0.45	0/1026
4	D	0.11	0/766	0.37	0/1026
4	H	0.13	0/756	0.34	0/1015
4	N	0.11	0/766	0.34	0/1026
4	R	0.13	0/756	0.34	0/1015
4	X	0.11	0/766	0.35	0/1026
4	d	0.16	0/756	0.39	0/1015
4	h	0.11	0/766	0.34	0/1026
4	n	0.20	0/756	0.36	0/1015
4	r	0.18	0/766	0.40	0/1026
4	x	0.13	0/756	0.35	0/1015
5	I	0.22	0/25620	0.47	0/39502
6	J	0.22	0/25990	0.49	12/40152 (0.0%)
All	All	0.20	0/88210	0.44	13/128794 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1048	DG	OP2-P-O3'	-9.36	79.92	108.00
6	J	300	DG	OP2-P-O3'	-9.30	80.10	108.00
6	J	861	DG	OP2-P-O3'	-9.30	80.10	108.00
6	J	487	DG	OP2-P-O3'	-9.29	80.14	108.00
6	J	674	DG	OP2-P-O3'	-9.25	80.25	108.00

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	801	0	839	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	807	0	844	27	0
1	K	801	0	839	36	0
1	O	807	0	844	23	0
1	U	801	0	839	33	0
1	Y	807	0	844	36	0
1	a	807	0	844	18	0
1	e	801	0	839	31	0
1	k	807	0	844	47	0
1	o	801	0	839	41	0
1	u	807	0	844	25	0
1	y	801	0	839	10	0
2	B	653	0	696	20	15
2	F	653	0	696	16	0
2	L	653	0	696	22	0
2	P	653	0	696	14	0
2	V	653	0	696	31	0
2	Z	653	0	696	26	4
2	b	653	0	696	15	15
2	f	653	0	696	22	0
2	l	653	0	696	43	0
2	p	653	0	696	39	0
2	v	653	0	696	10	0
2	z	653	0	696	10	0
3	0	810	0	866	38	0
3	2	796	0	848	37	1
3	C	796	0	848	15	0
3	G	810	0	866	28	0
3	M	796	0	848	21	0
3	Q	810	0	866	31	0
3	W	796	0	848	26	0
3	c	810	0	866	45	0
3	g	796	0	848	26	0
3	m	810	0	866	43	0
3	q	796	0	848	33	0
3	w	810	0	866	38	0
4	1	745	0	771	15	0
4	3	755	0	784	17	3
4	D	755	0	784	6	0
4	H	745	0	771	23	0
4	N	755	0	784	15	0
4	R	745	0	771	22	0
4	X	755	0	784	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	745	0	771	26	0
4	h	755	0	784	22	0
4	n	745	0	771	25	0
4	r	755	0	784	33	0
4	x	745	0	771	21	0
5	I	22861	0	12579	610	0
6	J	23141	0	12584	673	0
All	All	82122	0	63227	1824	19

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 13.

The worst 5 of 1824 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:132:DA:H5'	3:w:42:ARG:HG2	1.32	1.08
1:o:76:GLN:OE1	2:p:22:LEU:HD12	1.55	1.05
2:l:98:TYR:HB3	4:r:58:ILE:HG13	1.40	1.03
2:V:92:ARG:HH21	4:X:98:LEU:HA	1.25	1.02
6:J:505:DG:H4'	3:m:42:ARG:HB3	1.43	0.98

The worst 5 of 19 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:B:23:ARG:CG	2:b:23:ARG:CG[3_455]	0.58	1.62
2:B:23:ARG:CD	2:b:23:ARG:CG[3_455]	1.01	1.19
2:B:23:ARG:CG	2:b:23:ARG:CD[3_455]	1.01	1.19
2:B:23:ARG:CB	2:b:23:ARG:CD[3_455]	1.52	0.68
2:B:23:ARG:CD	2:b:23:ARG:CB[3_455]	1.53	0.67

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	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	E	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	K	95/139 (68%)	91 (96%)	4 (4%)	0	100	100
1	O	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	U	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	Y	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	a	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	e	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	k	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	o	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
1	u	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	y	87/139 (63%)	85 (98%)	2 (2%)	0	100	100
2	B	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	F	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	L	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	P	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	V	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	Z	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	b	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	f	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	l	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	p	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	v	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	z	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
3	0	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	2	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	C	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	G	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	M	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	Q	103/133 (77%)	102 (99%)	1 (1%)	0	100	100
3	W	101/133 (76%)	100 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	103/133 (77%)	102 (99%)	1 (1%)	0	100	100
3	g	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	m	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	q	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
3	w	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
4	1	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	3	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	D	94/129 (73%)	89 (95%)	4 (4%)	1 (1%)	11	46
4	H	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	N	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	R	93/129 (72%)	92 (99%)	0	1 (1%)	11	46
4	X	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	d	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	h	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	n	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	r	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	x	93/129 (72%)	92 (99%)	0	1 (1%)	11	46
All	All	4444/6084 (73%)	4342 (98%)	90 (2%)	12 (0%)	36	72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	H	101	GLY
4	d	101	GLY
4	h	101	GLY
4	N	101	GLY

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	85/113 (75%)	85 (100%)	0	100	100
1	E	85/113 (75%)	85 (100%)	0	100	100
1	K	85/113 (75%)	85 (100%)	0	100	100
1	O	85/113 (75%)	85 (100%)	0	100	100
1	U	85/113 (75%)	85 (100%)	0	100	100
1	Y	85/113 (75%)	85 (100%)	0	100	100
1	a	85/113 (75%)	85 (100%)	0	100	100
1	e	85/113 (75%)	85 (100%)	0	100	100
1	k	85/113 (75%)	85 (100%)	0	100	100
1	o	85/113 (75%)	85 (100%)	0	100	100
1	u	85/113 (75%)	85 (100%)	0	100	100
1	y	85/113 (75%)	85 (100%)	0	100	100
2	B	67/81 (83%)	67 (100%)	0	100	100
2	F	67/81 (83%)	67 (100%)	0	100	100
2	L	67/81 (83%)	67 (100%)	0	100	100
2	P	67/81 (83%)	67 (100%)	0	100	100
2	V	67/81 (83%)	67 (100%)	0	100	100
2	Z	67/81 (83%)	67 (100%)	0	100	100
2	b	67/81 (83%)	67 (100%)	0	100	100
2	f	67/81 (83%)	67 (100%)	0	100	100
2	l	67/81 (83%)	67 (100%)	0	100	100
2	p	67/81 (83%)	67 (100%)	0	100	100
2	v	67/81 (83%)	67 (100%)	0	100	100
2	z	67/81 (83%)	67 (100%)	0	100	100
3	0	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	2	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	C	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	G	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	M	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	Q	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	W	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	c	83/102 (81%)	81 (98%)	2 (2%)	43	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	g	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	m	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	q	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	w	83/102 (81%)	81 (98%)	2 (2%)	43	64
4	1	81/107 (76%)	80 (99%)	1 (1%)	63	75
4	3	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	D	82/107 (77%)	82 (100%)	0	100	100
4	H	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	N	82/107 (77%)	82 (100%)	0	100	100
4	R	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	X	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	d	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	h	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	n	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	r	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	x	81/107 (76%)	79 (98%)	2 (2%)	42	63
All	All	3792/4836 (78%)	3753 (99%)	39 (1%)	68	78

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	X	85	THR
4	x	103	LEU
3	0	62	ILE
3	w	62	ILE
3	2	81	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
4	R	92	GLN
1	u	108	ASN
3	m	94	ASN
3	2	31	HIS
2	V	25	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

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, 95th 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 ²)	Q<0.9
1	A	97/139 (69%)	-0.79	0 100 100	321, 473, 538, 576	0
1	E	98/139 (70%)	-0.62	1 (1%) 79 68	379, 442, 554, 584	0
1	K	97/139 (69%)	-0.63	0 100 100	363, 424, 476, 499	0
1	O	98/139 (70%)	-0.52	0 100 100	403, 468, 528, 545	0
1	U	97/139 (69%)	-0.70	1 (1%) 79 68	382, 448, 493, 535	0
1	Y	98/139 (70%)	-0.57	0 100 100	400, 463, 530, 547	0
1	a	98/139 (70%)	-0.76	0 100 100	362, 467, 535, 568	0
1	e	97/139 (69%)	-0.76	0 100 100	404, 464, 549, 627	0
1	k	98/139 (70%)	-0.68	0 100 100	331, 420, 462, 473	0
1	o	97/139 (69%)	-0.84	0 100 100	336, 416, 471, 508	0
1	u	98/139 (70%)	-0.58	0 100 100	358, 445, 515, 546	0
1	y	97/139 (69%)	-0.67	2 (2%) 63 54	424, 502, 578, 608	0
2	B	82/106 (77%)	-0.69	0 100 100	392, 470, 528, 565	0
2	F	82/106 (77%)	-0.85	0 100 100	366, 429, 480, 492	0
2	L	82/106 (77%)	-0.58	2 (2%) 59 52	379, 427, 464, 472	0
2	P	82/106 (77%)	-0.53	2 (2%) 59 52	390, 469, 529, 597	0
2	V	82/106 (77%)	-0.50	0 100 100	349, 414, 457, 490	0
2	Z	82/106 (77%)	-0.56	0 100 100	353, 454, 504, 522	0
2	b	82/106 (77%)	-0.81	1 (1%) 76 65	385, 460, 501, 582	0
2	f	82/106 (77%)	-0.28	2 (2%) 59 52	369, 474, 538, 568	0
2	l	82/106 (77%)	-0.73	0 100 100	365, 408, 453, 463	0
2	p	82/106 (77%)	-0.82	0 100 100	323, 411, 488, 502	0
2	v	82/106 (77%)	-0.63	0 100 100	375, 440, 490, 512	0
2	z	82/106 (77%)	-0.78	0 100 100	415, 487, 533, 550	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	0	105/133 (78%)	-0.47	0 100 100	415, 471, 522, 539	0
3	2	103/133 (77%)	-0.54	0 100 100	386, 439, 519, 589	0
3	C	103/133 (77%)	-0.54	0 100 100	366, 456, 499, 562	0
3	G	105/133 (78%)	-0.71	0 100 100	284, 478, 544, 590	0
3	M	103/133 (77%)	-0.33	2 (1%) 66 56	355, 450, 510, 524	0
3	Q	105/133 (78%)	-0.41	1 (0%) 79 68	357, 430, 493, 512	0
3	W	103/133 (77%)	-0.12	3 (2%) 53 47	360, 451, 538, 596	0
3	c	105/133 (78%)	-0.16	1 (0%) 79 68	407, 479, 585, 614	0
3	g	103/133 (77%)	-0.71	0 100 100	328, 472, 527, 546	0
3	m	105/133 (78%)	-0.42	1 (0%) 79 68	339, 467, 515, 551	0
3	q	103/133 (77%)	-0.31	2 (1%) 66 56	343, 421, 472, 500	0
3	w	105/133 (78%)	-0.71	0 100 100	439, 512, 584, 603	0
4	1	95/129 (73%)	-0.15	3 (3%) 50 45	409, 471, 529, 551	0
4	3	96/129 (74%)	-0.34	0 100 100	371, 443, 518, 590	0
4	D	96/129 (74%)	-0.60	1 (1%) 79 68	366, 440, 512, 547	0
4	H	95/129 (73%)	-0.55	1 (1%) 78 67	405, 463, 569, 620	0
4	N	96/129 (74%)	-0.20	3 (3%) 51 46	365, 453, 518, 551	0
4	R	95/129 (73%)	-0.46	0 100 100	361, 433, 484, 539	0
4	X	96/129 (74%)	-0.10	3 (3%) 51 46	364, 430, 501, 538	0
4	d	95/129 (73%)	-0.09	1 (1%) 78 67	415, 475, 540, 557	0
4	h	96/129 (74%)	-0.55	0 100 100	397, 491, 554, 609	0
4	n	95/129 (73%)	-0.09	6 (6%) 26 31	410, 460, 514, 555	0
4	r	96/129 (74%)	-0.25	2 (2%) 63 54	349, 433, 493, 551	0
4	x	95/129 (73%)	-0.50	0 100 100	414, 523, 592, 636	0
5	I	1122/1122 (100%)	-0.42	2 (0%) 91 84	378, 585, 848, 1000	0
6	J	1122/1122 (100%)	-0.45	0 100 100	441, 585, 866, 1000	0
All	All	6792/8328 (81%)	-0.49	43 (0%) 85 76	284, 481, 718, 1000	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	n	70	ILE	5.7
4	N	59	MET	4.7

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Mol	Chain	Res	Type	RSRZ
4	X	59	MET	3.7
4	D	59	MET	3.6
4	X	38	VAL	3.3

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.