



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:15 AM UTC

PDB ID : 7XVL / pdb_00007xvl
Title : Crystal Structure of Nucleosome-H1.0 Linker Histone Assembly (sticky-169an DNA fragment)
Authors : Adhireksan, Z.; Qiuye, B.; Lee, P.L.; Sharma, D.; Padavattan, S.; Davey, C.A.
Deposited on : 2022-05-24
Resolution : 3.51 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

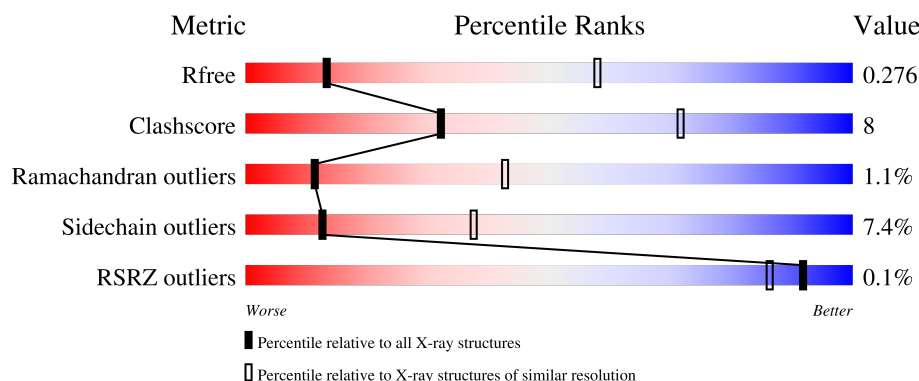
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	138	
1	E	138	
1	K	138	
1	O	138	
1	U	138	

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Mol	Chain	Length	Quality of chain
1	Y	138	
1	e	138	
1	i	138	
2	B	105	
2	F	105	
2	L	105	
2	P	105	
2	V	105	
2	Z	105	
2	f	105	
2	j	105	
3	C	132	
3	G	132	
3	M	132	
3	Q	132	
3	W	132	
3	a	132	
3	g	132	
3	k	132	
4	D	128	
4	H	128	
4	N	128	
4	R	128	
4	X	128	
4	b	128	

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Mol	Chain	Length	Quality of chain
4	h	128	
4	l	128	
5	I	169	
5	S	169	
5	c	169	
5	m	169	
6	J	169	
6	T	169	
6	d	169	
6	n	169	
7	o	195	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 52574 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	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	E	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	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	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	e	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	i	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P68431
A	-1	SER	-	expression tag	UNP P68431
E	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
K	-2	GLY	-	expression tag	UNP P68431
K	-1	SER	-	expression tag	UNP P68431
O	-2	GLY	-	expression tag	UNP P68431
O	-1	SER	-	expression tag	UNP P68431
U	-2	GLY	-	expression tag	UNP P68431
U	-1	SER	-	expression tag	UNP P68431
Y	-2	GLY	-	expression tag	UNP P68431
Y	-1	SER	-	expression tag	UNP P68431
e	-2	GLY	-	expression tag	UNP P68431

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Chain	Residue	Modelled	Actual	Comment	Reference
e	-1	SER	-	expression tag	UNP P68431
i	-2	GLY	-	expression tag	UNP P68431
i	-1	SER	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			
2	L	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	P	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
2	V	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	Z	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			
2	f	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	j	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62805
B	-1	SER	-	expression tag	UNP P62805
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
L	-2	GLY	-	expression tag	UNP P62805
L	-1	SER	-	expression tag	UNP P62805
P	-2	GLY	-	expression tag	UNP P62805
P	-1	SER	-	expression tag	UNP P62805
V	-2	GLY	-	expression tag	UNP P62805
V	-1	SER	-	expression tag	UNP P62805
Z	-2	GLY	-	expression tag	UNP P62805
Z	-1	SER	-	expression tag	UNP P62805
f	-2	GLY	-	expression tag	UNP P62805
f	-1	SER	-	expression tag	UNP P62805
j	-2	GLY	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
j	-1	SER	-	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	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	G	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	M	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	Q	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	W	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	a	104	Total	C	N	O	0	0	0
			805	508	157	140			
3	g	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	k	104	Total	C	N	O	0	0	0
			805	508	157	140			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04908
C	-1	SER	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
M	-2	GLY	-	expression tag	UNP P04908
M	-1	SER	-	expression tag	UNP P04908
Q	-2	GLY	-	expression tag	UNP P04908
Q	-1	SER	-	expression tag	UNP P04908
W	-2	GLY	-	expression tag	UNP P04908
W	-1	SER	-	expression tag	UNP P04908
a	-2	GLY	-	expression tag	UNP P04908
a	-1	SER	-	expression tag	UNP P04908
g	-2	GLY	-	expression tag	UNP P04908
g	-1	SER	-	expression tag	UNP P04908
k	-2	GLY	-	expression tag	UNP P04908
k	-1	SER	-	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	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	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	b	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
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			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
H	-2	GLY	-	expression tag	UNP P06899
H	-1	SER	-	expression tag	UNP P06899
N	-2	GLY	-	expression tag	UNP P06899
N	-1	SER	-	expression tag	UNP P06899
R	-2	GLY	-	expression tag	UNP P06899
R	-1	SER	-	expression tag	UNP P06899
X	-2	GLY	-	expression tag	UNP P06899
X	-1	SER	-	expression tag	UNP P06899
b	-2	GLY	-	expression tag	UNP P06899
b	-1	SER	-	expression tag	UNP P06899
h	-2	GLY	-	expression tag	UNP P06899
h	-1	SER	-	expression tag	UNP P06899
l	-2	GLY	-	expression tag	UNP P06899
l	-1	SER	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	169	Total	C	N	O	P	0	0	0
			3457	1639	656	993	169			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S	169	Total	C	N	O	P	0	0	0
			3457	1639	656	993	169			
5	c	169	Total	C	N	O	P	0	0	0
			3457	1639	656	993	169			
5	m	169	Total	C	N	O	P	0	0	0
			3457	1639	656	993	169			

- Molecule 6 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	169	Total	C	N	O	P	0	0	0
			3474	1652	616	1037	169			
6	T	169	Total	C	N	O	P	0	0	0
			3474	1652	616	1037	169			
6	d	169	Total	C	N	O	P	0	0	0
			3474	1652	616	1037	169			
6	n	169	Total	C	N	O	P	0	0	0
			3474	1652	616	1037	169			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	o	78	Total	C	N	O	S	0	0	0
			595	368	111	115	1			

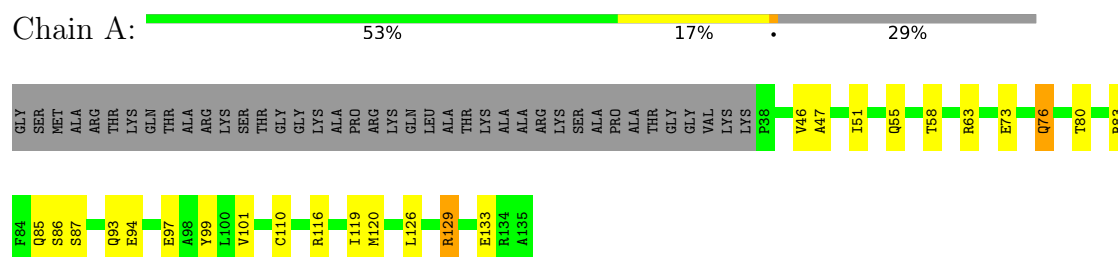
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	0	GLY	-	expression tag	UNP P07305
o	1	PRO	-	expression tag	UNP P07305

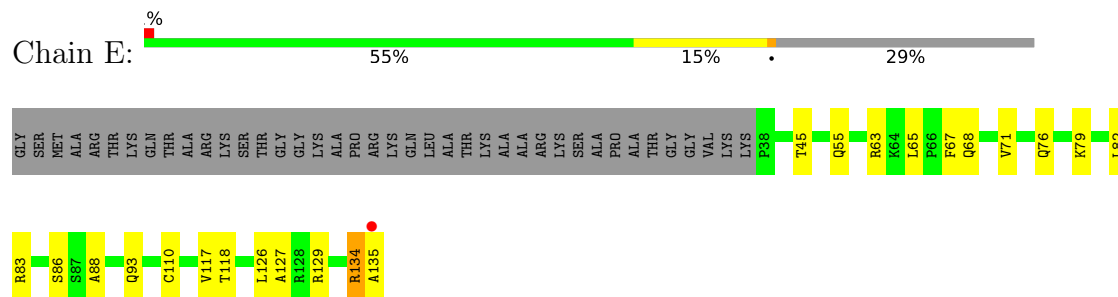
3 Residue-property plots [i](#)

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.

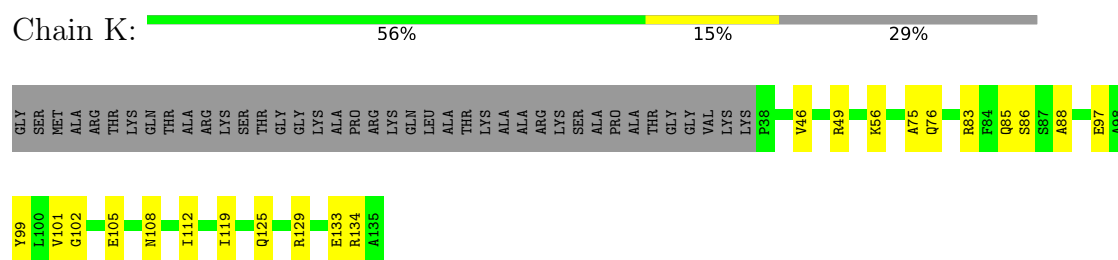
• Molecule 1: Histone H3.1



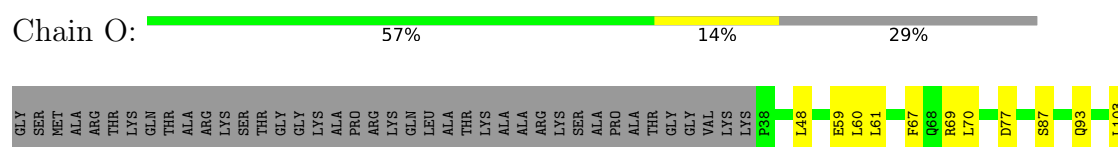
• Molecule 1: Histone H3.1



• Molecule 1: Histone H3.1



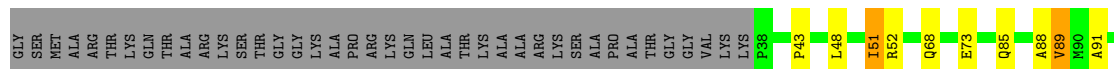
• Molecule 1: Histone H3.1





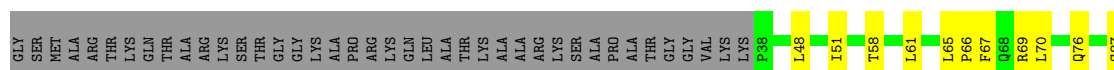
- Molecule 1: Histone H3.1

Chain U: 59% 11% 29%



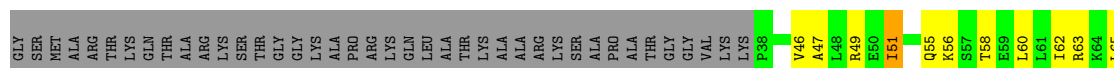
- Molecule 1: Histone H3.1

Chain Y: 54% 17% 29%



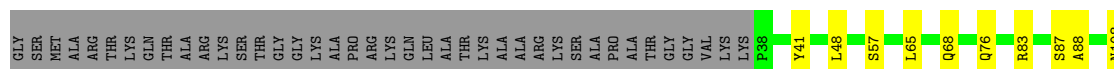
- Molecule 1: Histone H3.1

Chain e: 53% 17% 29%



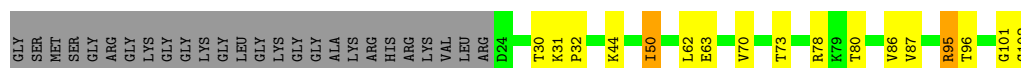
- Molecule 1: Histone H3.1

Chain i: 59% 12% 29%



- Molecule 2: Histone H4

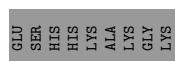
Chain B: 59% 14% 25%



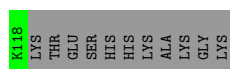
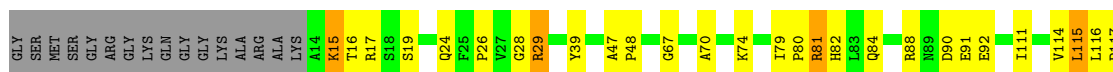
- Chain j: 62% 13% . 24%



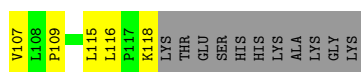
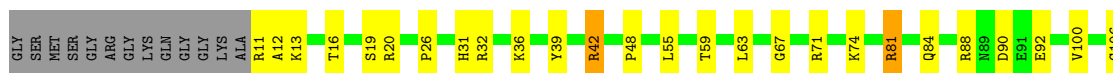
- Molecule 3: Histone H2A type 1-B/E



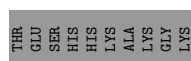
- Molecule 3: Histone H2A type 1-B/E



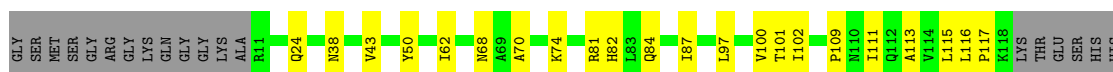
- Molecule 3: Histone H2A type 1-B/E



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



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



LYS
ALA
LYS
GLY
LYS

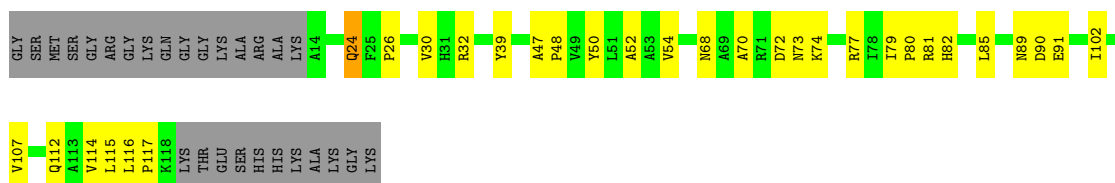
• Molecule 3: Histone H2A type 1-B/E

Chain a: 55% 22% • 21%



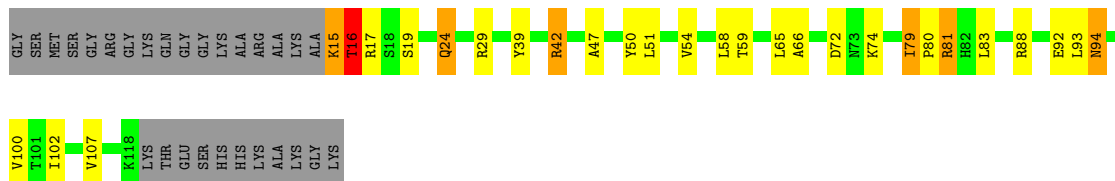
• Molecule 3: Histone H2A type 1-B/E

Chain g: 56% 23% • 20%



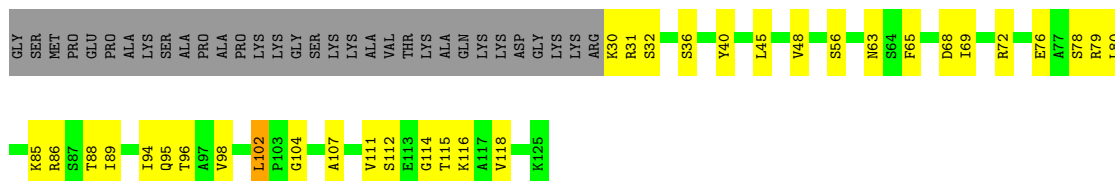
• Molecule 3: Histone H2A type 1-B/E

Chain k: 57% 17% 5% • 21%



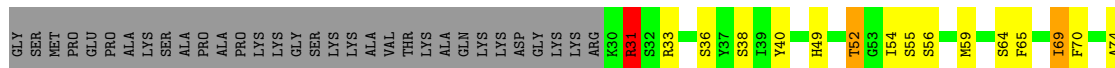
• Molecule 4: Histone H2B type 1-J

Chain D: 48% 26% • 25%



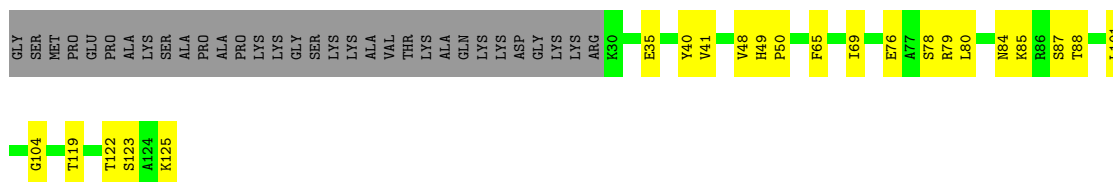
• Molecule 4: Histone H2B type 1-J

Chain H: 47% 25% •• 25%

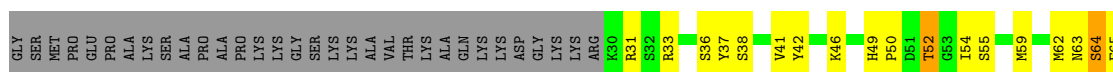




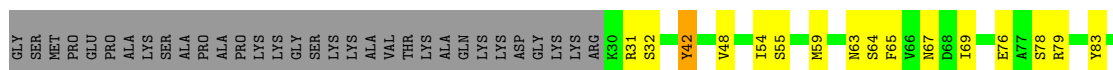
• Molecule 4: Histone H2B type 1-J



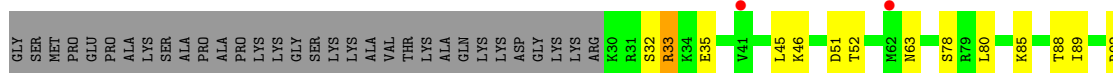
• Molecule 4: Histone H2B type 1-J



• Molecule 4: Histone H2B type 1-J

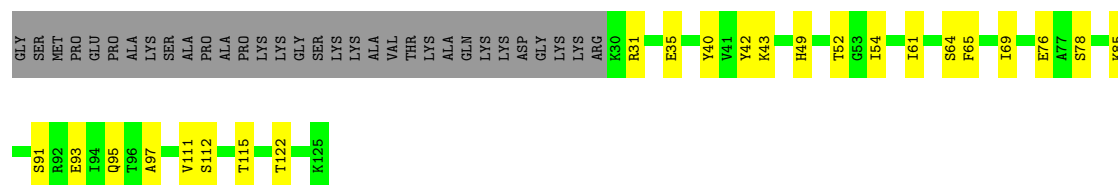


• Molecule 4: Histone H2B type 1-J

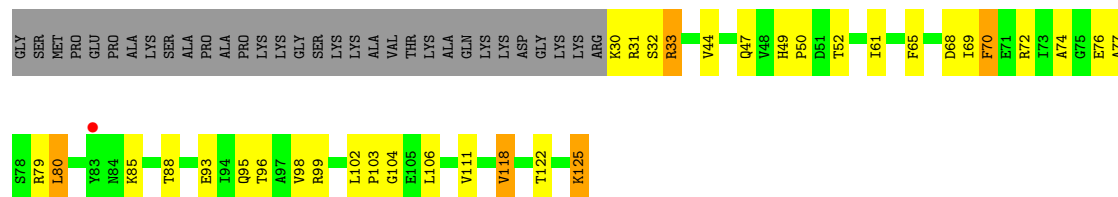


• Molecule 4: Histone H2B type 1-J

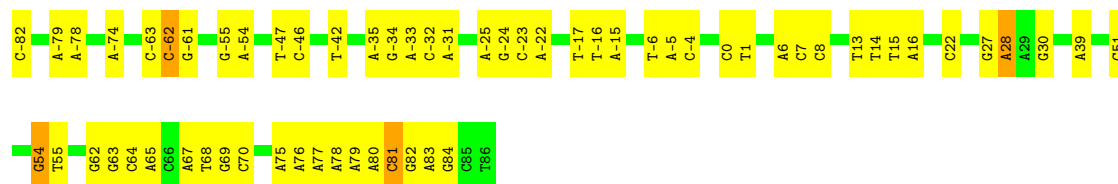




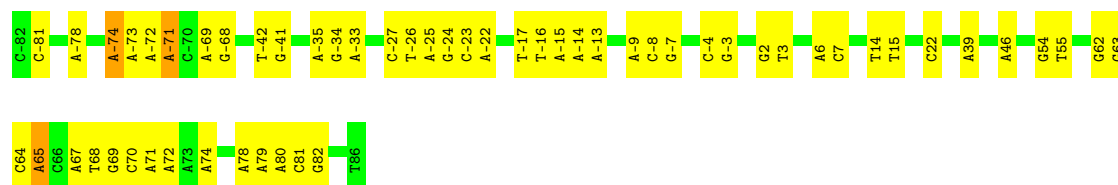
• Molecule 4: Histone H2B type 1-J



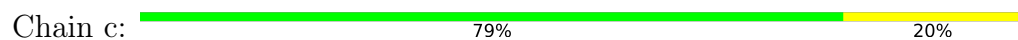
• Molecule 5: DNA (169-MER)



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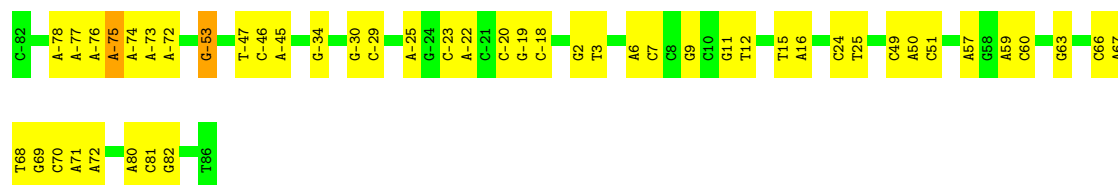


• Molecule 5: DNA (169-MER)

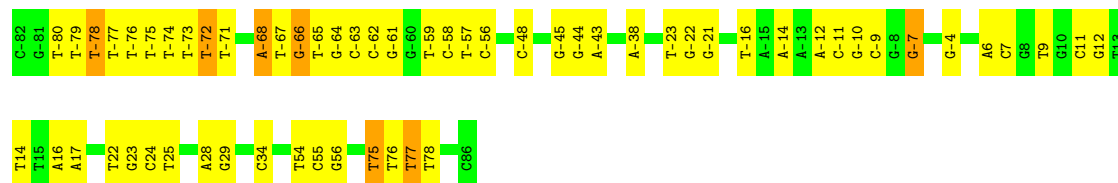


• Molecule 5: DNA (169-MER)

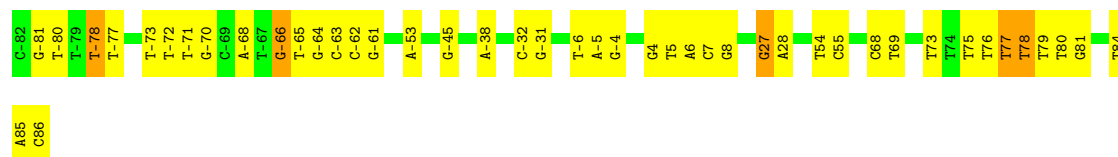




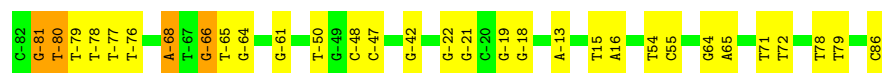
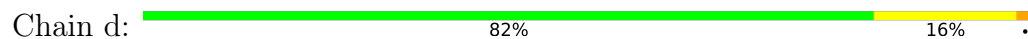
- Molecule 6: DNA (169-MER)



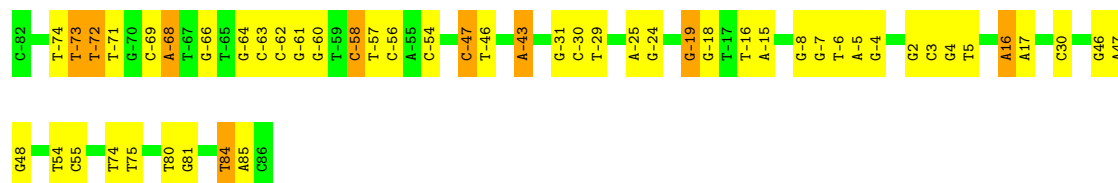
- Molecule 6: DNA (169-MER)



- Molecule 6: DNA (169-MER)



- Molecule 6: DNA (169-MER)



- Molecule 7: Histone H1.0



Lys	Lys	ALA	L70
		PRO	S71
Lys	Lys	THR	L72
		LYS	K73
Lys	Lys	PRO	R74
		ALA	L75
Lys	Lys	ALA	V76
		THR	V80
Lys	Lys	PRO	L81
		VAL	K82
Lys	Lys	LYS	Q83
		ALA	T84
Lys	Lys	ALA	V87
		LYS	G88
Lys	Lys	LYS	A89
		LEU	S90
Lys	Lys	ALA	G91
		ALA	S92
Lys	Lys	THR	F93
		PRO	R94
Lys	Lys	LYS	L95
		LYS	A96
Lys	Lys	ALA	K97
		LYS	S98
Lys	Lys	PRO	D99
		LYS	GLU
Lys	Lys	LYS	PRO
		THR	LYS
Lys	Lys	VAL	LYS
		LYS	SER
Lys	Lys	ALA	VAL
		LYS	ALA
Lys	Lys	PRO	PHE
		VAL	LYS
Lys	Lys	LYS	LYS
		ALA	THR
Lys	Lys	SER	LYS
		LYS	LYS
Lys	Lys	PRO	GLU
		LYS	ILE
Lys	Lys	LYS	LYS
		ALA	LYS
Lys	Lys	PRO	VAL
		VAL	ALA
Lys	Lys	LYS	THR
		PRO	PRO
Lys	Lys	LYS	LYS
		ALA	LYS
Lys	Lys	ALA	ALA
		ARG	ALA
Lys	Lys	GLY	ALA
		LYS	LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	213.85Å 102.46Å 218.29Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	88.44 – 3.51 88.44 – 3.51	Depositor EDS
% Data completeness (in resolution range)	95.9 (88.44-3.51) 95.9 (88.44-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.280 0.209 , 0.276	Depositor DCC
R_{free} test set	2266 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	116.3	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52574	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% 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 ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	0/819	1.48	2/1097 (0.2%)
1	E	0.99	0/819	1.49	3/1097 (0.3%)
1	K	0.97	0/819	1.44	0/1097
1	O	0.98	0/819	1.48	0/1097
1	U	1.01	0/819	1.45	1/1097 (0.1%)
1	Y	0.99	0/819	1.51	0/1097
1	e	0.98	0/819	1.50	0/1097
1	i	0.98	0/819	1.46	0/1097
2	B	1.03	0/634	1.44	1/848 (0.1%)
2	F	0.97	0/711	1.54	3/948 (0.3%)
2	L	0.98	0/634	1.50	0/848
2	P	0.99	0/669	1.53	5/894 (0.6%)
2	V	0.99	0/634	1.47	0/848
2	Z	1.07	0/711	1.57	2/948 (0.2%)
2	f	1.02	0/634	1.61	0/848
2	j	0.97	0/645	1.53	0/862
3	C	0.99	0/845	1.44	3/1139 (0.3%)
3	G	1.01	0/820	1.45	0/1107
3	M	1.00	0/845	1.41	0/1139
3	Q	0.99	0/820	1.55	0/1107
3	W	1.00	0/845	1.55	2/1139 (0.2%)
3	a	1.03	0/815	1.52	4/1100 (0.4%)
3	g	0.99	0/820	1.51	0/1107
3	k	0.96	0/815	1.47	1/1100 (0.1%)
4	D	1.00	0/766	1.50	0/1026
4	H	1.01	0/766	1.51	1/1026 (0.1%)
4	N	1.02	0/766	1.58	4/1026 (0.4%)
4	R	1.01	0/766	1.55	0/1026
4	X	1.04	0/766	1.56	0/1026
4	b	1.03	0/766	1.57	0/1026
4	h	1.01	0/766	1.54	0/1026
4	l	0.99	0/766	1.51	0/1026
5	I	0.46	0/3883	0.87	6/5983 (0.1%)
5	S	0.41	0/3883	0.85	5/5983 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	c	0.37	0/3883	0.80	6/5983 (0.1%)
5	m	0.40	0/3883	0.86	5/5983 (0.1%)
6	J	0.47	0/3891	0.95	18/6008 (0.3%)
6	T	0.44	0/3891	0.88	7/6008 (0.1%)
6	d	0.36	0/3891	0.83	4/6008 (0.1%)
6	n	0.42	0/3891	0.89	13/6008 (0.2%)
7	o	1.11	0/601	1.60	2/802 (0.2%)
All	All	0.74	0/56274	1.17	98/81732 (0.1%)

There are no bond length outliers.

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	n	-66	DG	C2'-C3'-O3'	8.95	124.92	111.50
6	J	-72	DT	C2'-C3'-O3'	-8.68	98.48	111.50
6	J	-66	DG	C2'-C3'-O3'	8.39	124.08	111.50
6	d	-81	DG	C2'-C3'-O3'	-7.65	100.02	111.50
6	T	-66	DG	C2'-C3'-O3'	7.43	122.65	111.50

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	807	0	844	17	0
1	E	807	0	844	10	0
1	K	807	0	844	14	0
1	O	807	0	844	10	0
1	U	807	0	844	16	0
1	Y	807	0	844	23	0
1	e	807	0	844	14	0
1	i	807	0	844	8	0
2	B	627	0	663	13	0
2	F	703	0	755	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	627	0	663	12	0
2	P	662	0	709	17	0
2	V	627	0	663	26	1
2	Z	703	0	755	31	1
2	f	627	0	663	13	0
2	j	638	0	676	10	0
3	C	835	0	897	17	0
3	G	810	0	866	33	0
3	M	835	0	897	26	1
3	Q	810	0	866	16	0
3	W	835	0	897	14	0
3	a	805	0	861	31	0
3	g	810	0	866	24	0
3	k	805	0	861	19	0
4	D	755	0	784	23	0
4	H	755	0	784	22	0
4	N	755	0	784	14	0
4	R	755	0	784	24	0
4	X	755	0	784	14	0
4	b	755	0	784	10	1
4	h	755	0	784	20	0
4	l	755	0	784	36	0
5	I	3457	0	1889	48	0
5	S	3457	0	1889	43	0
5	c	3457	0	1889	24	1
5	m	3457	0	1889	39	0
6	J	3474	0	1911	40	0
6	T	3474	0	1911	35	0
6	d	3474	0	1911	21	1
6	n	3474	0	1911	38	0
7	o	595	0	618	36	0
All	All	52574	0	41400	736	3

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 8.

The worst 5 of 736 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)
3:G:114:VAL:HG23	3:G:115:LEU:HD23	1.38	1.04
3:M:11:ARG:HG2	3:M:12:ALA:H	1.17	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:116:LEU:HB3	3:W:117:PRO:HD2	1.40	0.99
7:o:54:ILE:HD11	7:o:68:ILE:HD11	1.48	0.94
1:U:73:GLU:OE1	2:V:25:ASN:HB2	1.68	0.93

All (3) 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)
4:b:51:ASP:N	5:c:-61:DG:OP1[2_657]	1.93	0.27
3:M:13:LYS:NZ	6:d:-50:DT:O3'[2_657]	1.97	0.23
2:V:59:LYS:NZ	2:Z:17:ARG:CB[2_647]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	96/138 (70%)	88 (92%)	8 (8%)	0	100	100
1	E	96/138 (70%)	91 (95%)	5 (5%)	0	100	100
1	K	96/138 (70%)	86 (90%)	10 (10%)	0	100	100
1	O	96/138 (70%)	92 (96%)	4 (4%)	0	100	100
1	U	96/138 (70%)	87 (91%)	7 (7%)	2 (2%)	5	31
1	Y	96/138 (70%)	88 (92%)	8 (8%)	0	100	100
1	e	96/138 (70%)	89 (93%)	6 (6%)	1 (1%)	12	44
1	i	96/138 (70%)	88 (92%)	8 (8%)	0	100	100
2	B	77/105 (73%)	66 (86%)	11 (14%)	0	100	100
2	F	85/105 (81%)	71 (84%)	13 (15%)	1 (1%)	10	41
2	L	77/105 (73%)	66 (86%)	11 (14%)	0	100	100
2	P	81/105 (77%)	72 (89%)	8 (10%)	1 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	77/105 (73%)	68 (88%)	7 (9%)	2 (3%)	4	27
2	Z	85/105 (81%)	72 (85%)	10 (12%)	3 (4%)	3	23
2	f	77/105 (73%)	67 (87%)	10 (13%)	0	100	100
2	j	78/105 (74%)	69 (88%)	9 (12%)	0	100	100
3	C	106/132 (80%)	94 (89%)	12 (11%)	0	100	100
3	G	103/132 (78%)	92 (89%)	11 (11%)	0	100	100
3	M	106/132 (80%)	94 (89%)	11 (10%)	1 (1%)	14	47
3	Q	103/132 (78%)	95 (92%)	7 (7%)	1 (1%)	12	44
3	W	106/132 (80%)	92 (87%)	13 (12%)	1 (1%)	14	47
3	a	102/132 (77%)	88 (86%)	12 (12%)	2 (2%)	6	32
3	g	103/132 (78%)	87 (84%)	16 (16%)	0	100	100
3	k	102/132 (77%)	89 (87%)	11 (11%)	2 (2%)	6	32
4	D	94/128 (73%)	84 (89%)	8 (8%)	2 (2%)	5	31
4	H	94/128 (73%)	86 (92%)	6 (6%)	2 (2%)	5	31
4	N	94/128 (73%)	86 (92%)	7 (7%)	1 (1%)	11	43
4	R	94/128 (73%)	78 (83%)	12 (13%)	4 (4%)	2	18
4	X	94/128 (73%)	79 (84%)	13 (14%)	2 (2%)	5	31
4	b	94/128 (73%)	81 (86%)	11 (12%)	2 (2%)	5	31
4	h	94/128 (73%)	83 (88%)	10 (11%)	1 (1%)	11	43
4	l	94/128 (73%)	84 (89%)	8 (8%)	2 (2%)	5	31
7	o	76/195 (39%)	64 (84%)	10 (13%)	2 (3%)	4	27
All	All	3064/4219 (73%)	2716 (89%)	313 (10%)	35 (1%)	11	43

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	N	104	GLY
2	P	21	VAL
4	R	33	ARG
2	V	28	GLY
2	Z	22	LEU

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	85/112 (76%)	81 (95%)	4 (5%)	23	49
1	E	85/112 (76%)	78 (92%)	7 (8%)	10	34
1	K	85/112 (76%)	83 (98%)	2 (2%)	43	64
1	O	85/112 (76%)	80 (94%)	5 (6%)	18	44
1	U	85/112 (76%)	85 (100%)	0	100	100
1	Y	85/112 (76%)	82 (96%)	3 (4%)	32	57
1	e	85/112 (76%)	80 (94%)	5 (6%)	18	44
1	i	85/112 (76%)	79 (93%)	6 (7%)	13	38
2	B	64/80 (80%)	62 (97%)	2 (3%)	35	59
2	F	72/80 (90%)	69 (96%)	3 (4%)	26	52
2	L	64/80 (80%)	61 (95%)	3 (5%)	23	49
2	P	68/80 (85%)	63 (93%)	5 (7%)	13	37
2	V	64/80 (80%)	62 (97%)	2 (3%)	35	59
2	Z	72/80 (90%)	64 (89%)	8 (11%)	6	25
2	f	64/80 (80%)	59 (92%)	5 (8%)	11	36
2	j	65/80 (81%)	62 (95%)	3 (5%)	24	50
3	C	85/101 (84%)	81 (95%)	4 (5%)	23	49
3	G	83/101 (82%)	77 (93%)	6 (7%)	13	38
3	M	85/101 (84%)	79 (93%)	6 (7%)	13	38
3	Q	83/101 (82%)	75 (90%)	8 (10%)	8	30
3	W	85/101 (84%)	78 (92%)	7 (8%)	10	34
3	a	83/101 (82%)	79 (95%)	4 (5%)	23	49
3	g	83/101 (82%)	78 (94%)	5 (6%)	17	44
3	k	83/101 (82%)	73 (88%)	10 (12%)	5	23
4	D	82/106 (77%)	74 (90%)	8 (10%)	7	30
4	H	82/106 (77%)	68 (83%)	14 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	82/106 (77%)	78 (95%)	4 (5%)	22	48
4	R	82/106 (77%)	71 (87%)	11 (13%)	4	20
4	X	82/106 (77%)	72 (88%)	10 (12%)	5	22
4	b	82/106 (77%)	74 (90%)	8 (10%)	7	30
4	h	82/106 (77%)	75 (92%)	7 (8%)	10	34
4	l	82/106 (77%)	76 (93%)	6 (7%)	13	38
7	o	65/158 (41%)	53 (82%)	12 (18%)	1	9
All	All	2604/3350 (78%)	2411 (93%)	193 (7%)	13	37

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	17	ARG
2	f	96	THR
2	Z	27	GLN
4	b	85	LYS
4	h	64	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	110	ASN
3	k	73	ASN
4	X	67	ASN
3	k	24	GLN
7	o	83	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [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, 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	98/138 (71%)	-0.72	0 100 100	63, 88, 132, 174	0
1	E	98/138 (71%)	-0.72	1 (1%) 79 56	59, 84, 123, 147	0
1	K	98/138 (71%)	-0.72	0 100 100	90, 115, 155, 190	0
1	O	98/138 (71%)	-0.75	0 100 100	84, 116, 149, 189	0
1	U	98/138 (71%)	-0.55	0 100 100	101, 149, 191, 202	0
1	Y	98/138 (71%)	-0.53	0 100 100	118, 162, 210, 227	0
1	e	98/138 (71%)	-0.70	1 (1%) 79 56	78, 108, 152, 185	0
1	i	98/138 (71%)	-0.65	0 100 100	84, 109, 155, 185	0
2	B	79/105 (75%)	-0.69	0 100 100	60, 82, 114, 156	0
2	F	87/105 (82%)	-0.59	0 100 100	64, 82, 187, 217	0
2	L	79/105 (75%)	-0.59	0 100 100	84, 111, 137, 147	0
2	P	83/105 (79%)	-0.74	0 100 100	88, 115, 156, 224	0
2	V	79/105 (75%)	-0.57	1 (1%) 75 50	104, 141, 172, 185	0
2	Z	87/105 (82%)	-0.44	0 100 100	106, 159, 221, 253	0
2	f	79/105 (75%)	-0.67	0 100 100	84, 106, 138, 145	0
2	j	80/105 (76%)	-0.62	0 100 100	80, 105, 150, 179	0
3	C	108/132 (81%)	-0.70	0 100 100	63, 89, 127, 190	0
3	G	105/132 (79%)	-0.61	0 100 100	59, 85, 136, 184	0
3	M	108/132 (81%)	-0.48	0 100 100	90, 124, 178, 226	0
3	Q	105/132 (79%)	-0.55	0 100 100	91, 116, 159, 195	0
3	W	108/132 (81%)	-0.44	0 100 100	108, 152, 197, 250	0
3	a	104/132 (78%)	-0.30	0 100 100	119, 156, 208, 245	0
3	g	105/132 (79%)	-0.63	0 100 100	86, 109, 159, 186	0
3	k	104/132 (78%)	-0.69	0 100 100	84, 112, 150, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
4	D	96/128 (75%)	-0.69	0	100	100	64, 90, 145, 216	0
4	H	96/128 (75%)	-0.52	0	100	100	54, 88, 160, 183	0
4	N	96/128 (75%)	-0.42	0	100	100	92, 124, 179, 228	0
4	R	96/128 (75%)	-0.53	0	100	100	100, 127, 177, 200	0
4	X	96/128 (75%)	-0.47	0	100	100	121, 157, 206, 212	0
4	b	96/128 (75%)	-0.24	2 (2%)	63	38	121, 166, 207, 222	0
4	h	96/128 (75%)	-0.44	0	100	100	77, 115, 174, 212	0
4	l	96/128 (75%)	-0.54	1 (1%)	79	56	80, 113, 168, 231	0
5	I	169/169 (100%)	-0.52	0	100	100	89, 145, 240, 312	0
5	S	169/169 (100%)	-0.40	0	100	100	121, 186, 251, 316	0
5	c	169/169 (100%)	-0.28	0	100	100	158, 221, 301, 363	0
5	m	169/169 (100%)	-0.38	0	100	100	118, 178, 244, 290	0
6	J	169/169 (100%)	-0.49	0	100	100	99, 142, 254, 339	0
6	T	169/169 (100%)	-0.37	0	100	100	127, 186, 258, 295	0
6	d	169/169 (100%)	-0.27	0	100	100	162, 228, 285, 342	0
6	n	169/169 (100%)	-0.40	0	100	100	130, 183, 265, 338	0
7	o	78/195 (40%)	-0.41	0	100	100	152, 195, 239, 272	1 (1%)
All	All	4482/5571 (80%)	-0.52	6 (0%)	92	86	54, 135, 236, 363	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	b	62	MET	4.0
4	b	41	VAL	3.7
1	E	135	ALA	3.4
1	e	135	ALA	3.2
4	l	83	TYR	2.2

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.