



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID : 7XX6 / pdb_00007xx6
Title : Crystal Structure of Nucleosome-H1.0 Linker Histone Assembly (sticky-169a DNA fragment)
Authors : Adhireksan, Z.; Qiuye, B.; Lee, P.L.; Sharma, D.; Padavattan, S.; Davey, C.A.
Deposited on : 2022-05-28
Resolution : 3.39 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

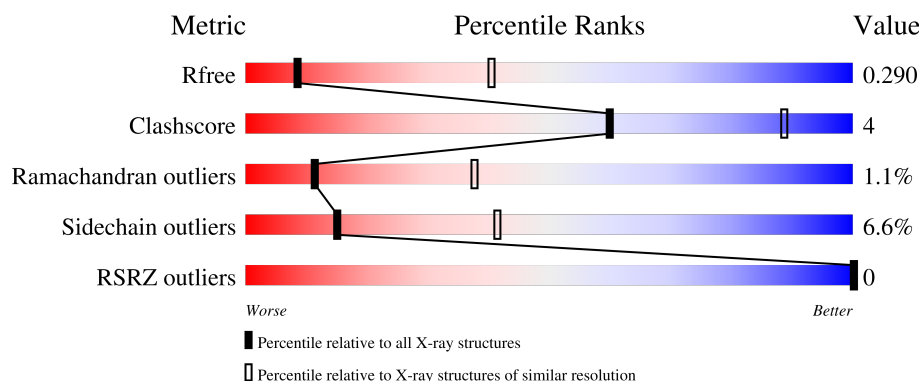
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	
7	p	195	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 53518 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	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	K	100	Total	C	N	O	S	0	0	0
			825	520	160	141	4			
1	O	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	U	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	Y	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	e	100	Total	C	N	O	S	0	0	0
			825	520	160	141	4			
1	i	99	Total	C	N	O	S	0	0	0
			816	514	158	140	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	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	F	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			
2	L	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	P	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	V	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	Z	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			
2	f	80	Total	C	N	O	S	0	0	0
			638	401	125	111	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	107	Total	C	N	O	0	0	0
			826	521	161	144			
3	G	114	Total	C	N	O	0	0	0
			873	549	173	151			
3	M	106	Total	C	N	O	0	0	0
			821	518	160	143			
3	Q	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	W	107	Total	C	N	O	0	0	0
			826	521	161	144			
3	a	114	Total	C	N	O	0	0	0
			873	549	173	151			
3	g	106	Total	C	N	O	0	0	0
			821	518	160	143			
3	k	105	Total	C	N	O	0	0	0
			810	511	158	141			

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	99	Total	C	N	O	S	0	0	0
			784	492	146	144	2			
4	H	99	Total	C	N	O	S	0	0	0
			784	492	146	144	2			
4	N	98	Total	C	N	O	S	0	0	0
			775	486	144	143	2			
4	R	98	Total	C	N	O	S	0	0	0
			775	486	144	143	2			
4	X	100	Total	C	N	O	S	0	0	0
			788	494	147	145	2			
4	b	100	Total	C	N	O	S	0	0	0
			788	494	147	145	2			
4	h	98	Total	C	N	O	S	0	0	0
			775	486	144	143	2			
4	l	98	Total	C	N	O	S	0	0	0
			775	486	144	143	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
			3462	1646	637	1011	168			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S	169	Total	C	N	O	P	0	0	0
			3462	1646	637	1011	168			
5	c	169	Total	C	N	O	P	0	0	0
			3462	1646	637	1011	168			
5	m	169	Total	C	N	O	P	0	0	0
			3462	1646	637	1011	168			

- 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
			3461	1646	634	1013	168			
6	T	169	Total	C	N	O	P	0	0	0
			3461	1646	634	1013	168			
6	d	169	Total	C	N	O	P	0	0	0
			3461	1646	634	1013	168			
6	n	169	Total	C	N	O	P	0	0	0
			3461	1646	634	1013	168			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	o	76	Total	C	N	O	S	0	0	0
			583	362	109	111	1			
7	p	74	Total	C	N	O	S	0	0	0
			566	353	107	105	1			

There are 4 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
p	0	GLY	-	expression tag	UNP P07305
p	1	PRO	-	expression tag	UNP P07305

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		
8	G	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	8	Total Ca 8 8	0	0
8	J	4	Total Ca 4 4	0	0
8	O	2	Total Ca 2 2	0	0
8	S	1	Total Ca 1 1	0	0
8	T	3	Total Ca 3 3	0	0
8	W	1	Total Ca 1 1	0	0
8	Y	1	Total Ca 1 1	0	0
8	a	2	Total Ca 2 2	0	0
8	c	7	Total Ca 7 7	0	0
8	d	8	Total Ca 8 8	0	0
8	i	1	Total Ca 1 1	0	0
8	j	1	Total Ca 1 1	0	0
8	m	2	Total Ca 2 2	0	0
8	n	2	Total Ca 2 2	0	0
8	o	1	Total Ca 1 1	0	0
8	p	1	Total Ca 1 1	0	0

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	1	Total K 1 1	0	0
9	T	3	Total K 3 3	0	0
9	c	1	Total K 1 1	0	0

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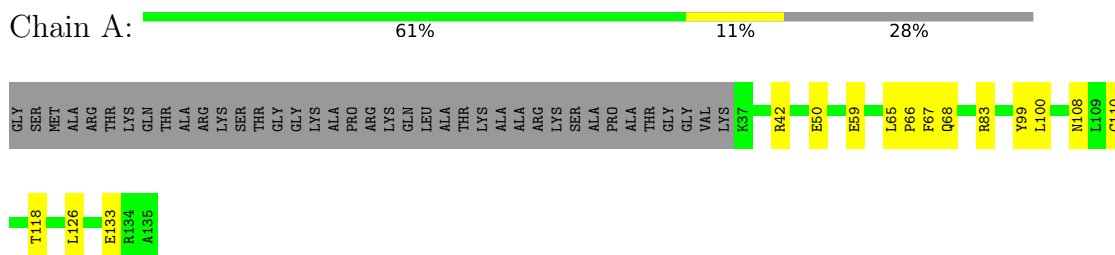
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	d	1	Total	K	0	0
			1	1		

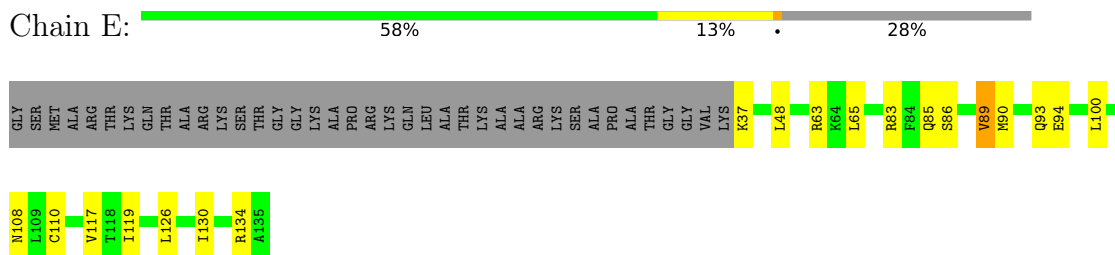
3 Residue-property plots [i](#)

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.

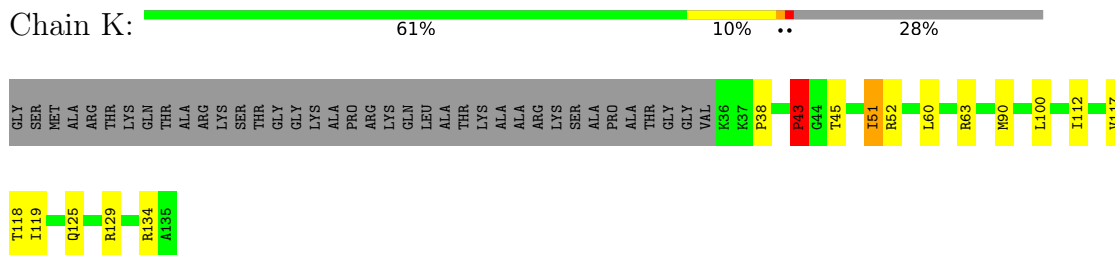
• Molecule 1: Histone H3.1



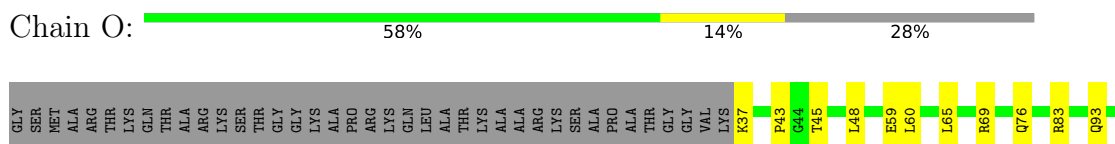
• Molecule 1: Histone H3.1



• Molecule 1: Histone H3.1



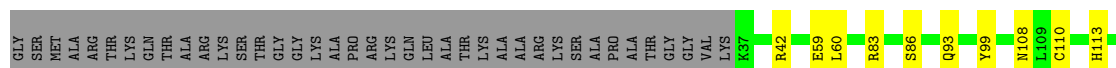
• Molecule 1: Histone H3.1





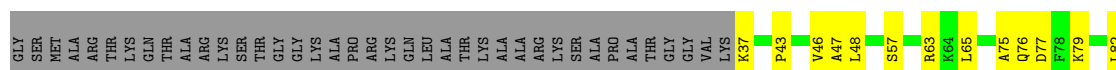
• Molecule 1: Histone H3.1

Chain U: 60% 12% 28%



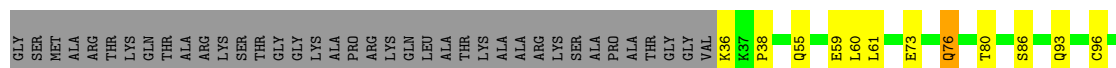
• Molecule 1: Histone H3.1

Chain Y: 54% 17% 28%



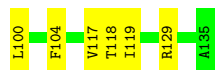
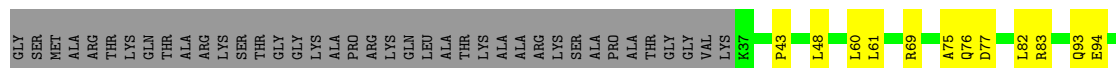
• Molecule 1: Histone H3.1

Chain e: 58% 14% 28%



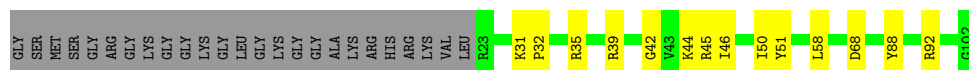
• Molecule 1: Histone H3.1

Chain i: 59% 13% 28%



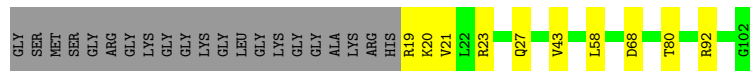
• Molecule 2: Histone H4

Chain B: 63% 13% 24%



- Molecule 2: Histone H4

Chain F:  70% 10% 20%



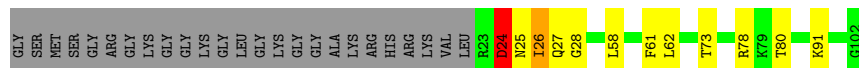
- Molecule 2: Histone H4

Chain L:  63% 12% 24%



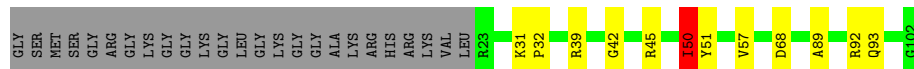
- Molecule 2: Histone H4

Chain P:  65% 10% 24%



- Molecule 2: Histone H4

Chain V:  65% 10% 24%



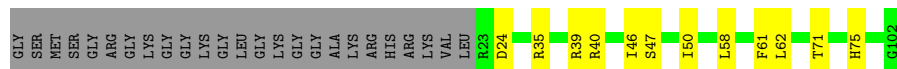
- Molecule 2: Histone H4

Chain Z:  65% 15% 20%



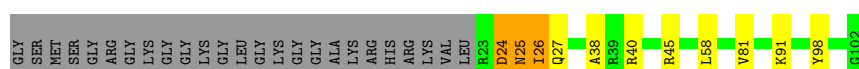
- Molecule 2: Histone H4

Chain f:  65% 11% 24%



- Molecule 2: Histone H4

Chain j:  66% 8% 24%



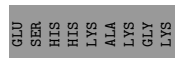
- Molecule 3: Histone H2A type 1-B/E

Chain C:  67% 13% 19%



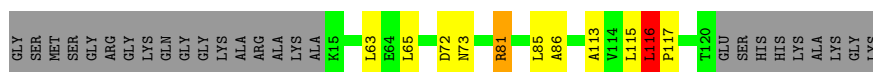
- Molecule 3: Histone H2A type 1-B/E

Chain G:  66% 18% 14%



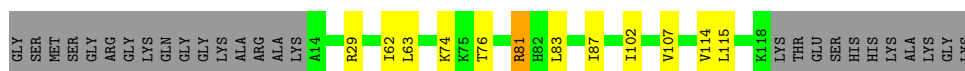
- Molecule 3: Histone H2A type 1-B/E

Chain M:  72% 7% 20%



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

Chain Q:  70% 8% 20%



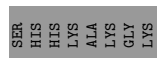
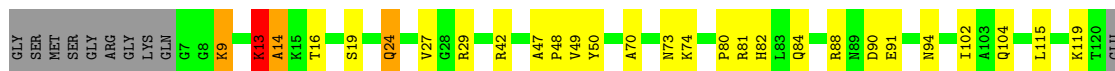
- Molecule 3: Histone H2A type 1-B/E

Chain W:  69% 11% 19%



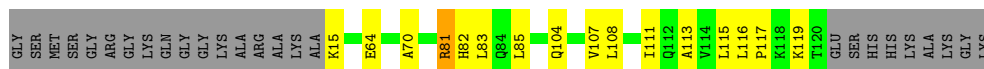
- Molecule 3: Histone H2A type 1-B/E

Chain a:  65% 18% 14%



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

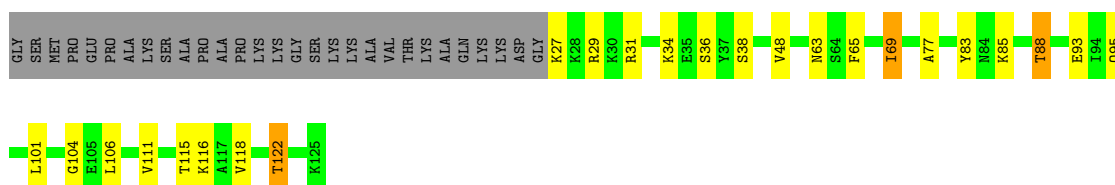
Chain g:  68% 11% 20%



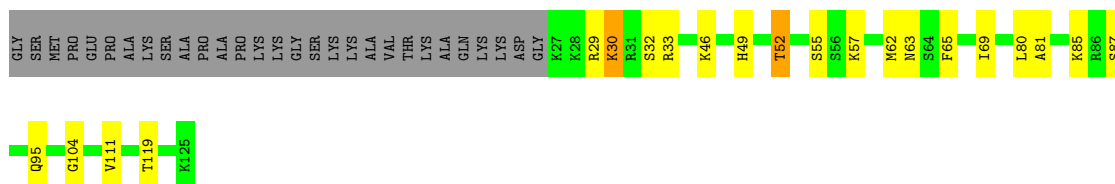
- Molecule 3: Histone H2A type 1-B/E



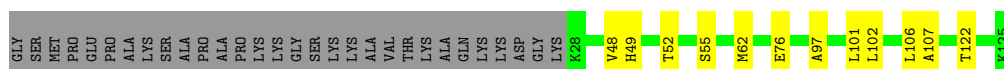
- Molecule 4: Histone H2B type 1-J



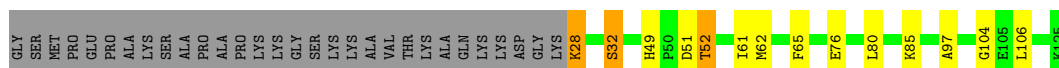
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J

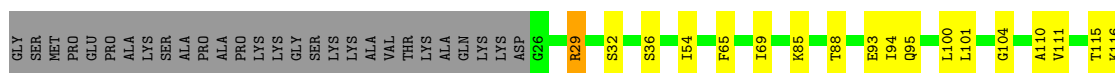


- Molecule 4: Histone H2B type 1-J

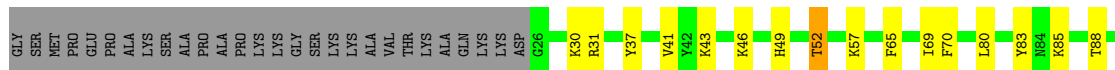


- Molecule 4: Histone H2B type 1-J





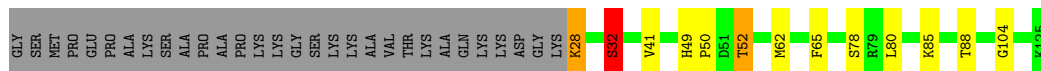
- Molecule 4: Histone H2B type 1-J



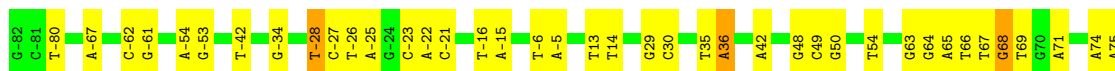
- Molecule 4: Histone H2B type 1-J



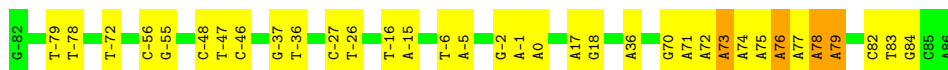
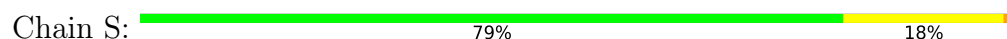
- Molecule 4: Histone H2B type 1-J



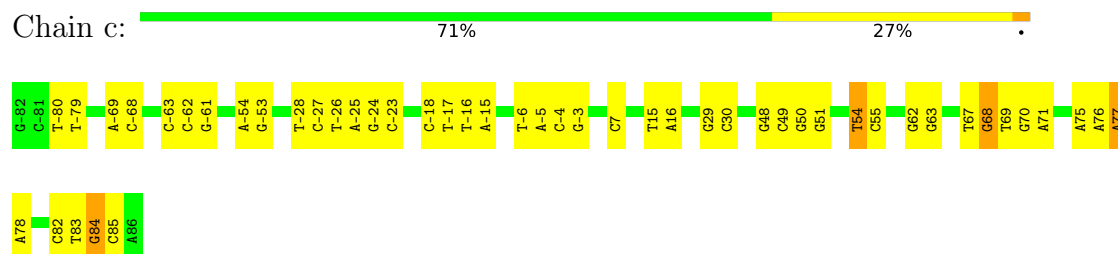
- Molecule 5: DNA (169-MER)



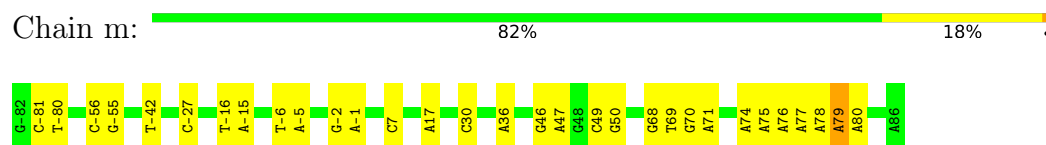
- Molecule 5: DNA (169-MER)



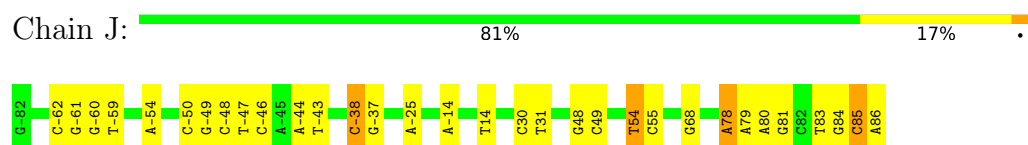
• Molecule 5: DNA (169-MER)



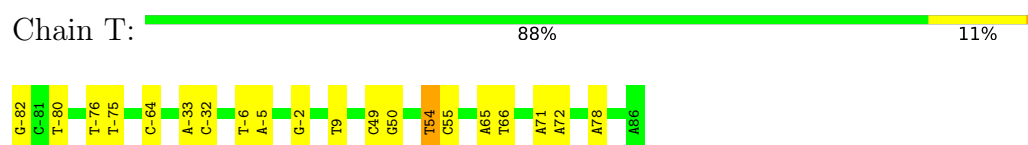
• Molecule 5: DNA (169-MER)



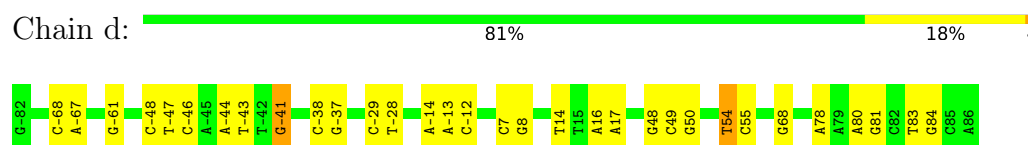
• Molecule 6: DNA (169-MER)



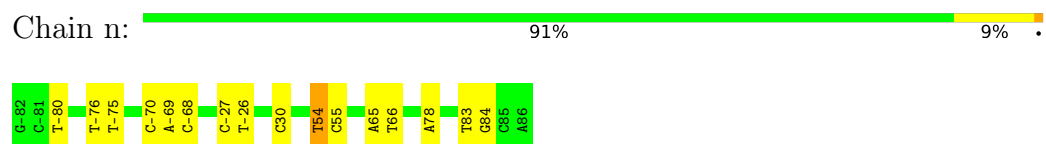
• Molecule 6: DNA (169-MER)



• Molecule 6: DNA (169-MER)

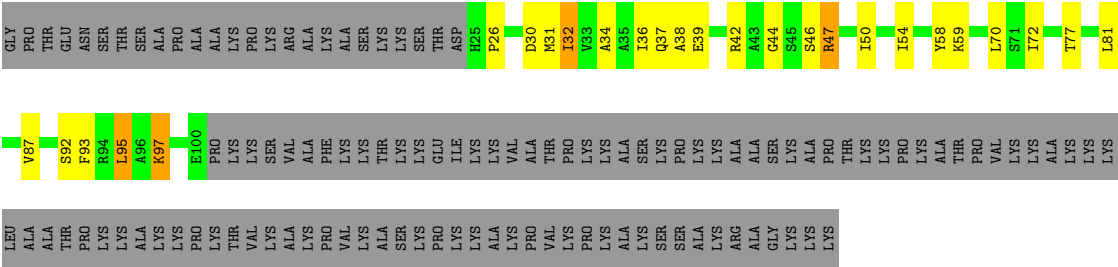


• Molecule 6: DNA (169-MER)

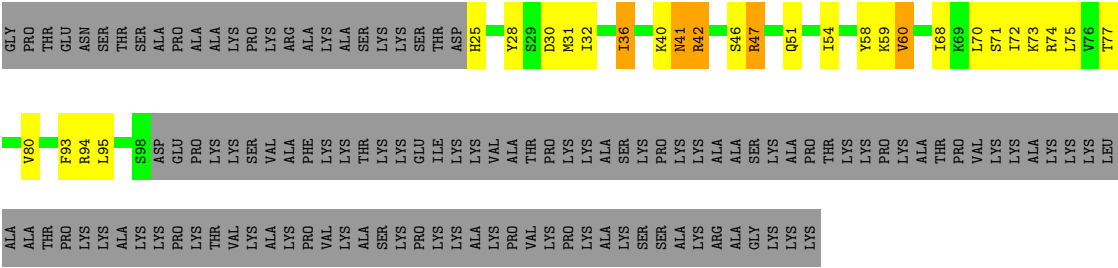


• Molecule 7: Histone H1.0





• 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, α , β , γ	208.78Å 102.37Å 212.71Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	48.83 – 3.39 48.83 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.83-3.39) 99.2 (48.83-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.227 , 0.296 0.230 , 0.290	Depositor DCC
R_{free} test set	2430 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	135.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 126.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53518	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9170e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, CA

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	0.74	0/828	1.04	0/1109
1	E	0.77	0/828	1.02	1/1109 (0.1%)
1	K	0.71	0/837	0.97	0/1120
1	O	0.76	0/828	0.99	0/1109
1	U	0.80	0/828	1.06	0/1109
1	Y	0.76	0/828	1.07	0/1109
1	e	0.71	0/837	0.93	1/1120 (0.1%)
1	i	0.75	0/828	0.95	0/1109
2	B	0.78	0/645	1.01	0/862
2	F	0.84	0/680	1.06	0/908
2	L	0.72	0/645	0.94	0/862
2	P	0.73	0/645	1.05	1/862 (0.1%)
2	V	0.85	0/645	1.09	1/862 (0.1%)
2	Z	0.82	0/680	1.06	0/908
2	f	0.71	0/645	0.99	0/862
2	j	0.73	0/645	0.98	0/862
3	C	0.71	0/836	1.06	1/1128 (0.1%)
3	G	0.84	1/883 (0.1%)	1.08	3/1188 (0.3%)
3	M	0.74	0/831	0.98	0/1121
3	Q	0.70	0/820	0.95	0/1107
3	W	0.71	0/836	1.05	1/1128 (0.1%)
3	a	0.84	0/883	1.04	0/1188
3	g	0.69	0/831	0.98	0/1121
3	k	0.68	0/820	0.94	0/1107
4	D	0.76	0/795	1.00	0/1062
4	H	0.76	0/795	1.10	0/1062
4	N	0.63	0/786	0.98	0/1051
4	R	0.65	0/786	0.99	0/1051
4	X	0.75	0/799	1.04	0/1067
4	b	0.76	0/799	1.05	0/1067
4	h	0.68	0/786	1.00	1/1051 (0.1%)
4	l	0.67	0/786	0.98	0/1051

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	I	0.41	0/3884	0.89	11/5993 (0.2%)
5	S	0.35	0/3884	0.83	6/5993 (0.1%)
5	c	0.43	0/3884	0.88	6/5993 (0.1%)
5	m	0.35	0/3884	0.81	3/5993 (0.1%)
6	J	0.42	0/3882	0.87	6/5990 (0.1%)
6	T	0.34	0/3882	0.81	4/5990 (0.1%)
6	d	0.42	0/3882	0.89	7/5990 (0.1%)
6	n	0.35	0/3882	0.80	3/5990 (0.1%)
7	o	1.01	0/589	1.14	4/785 (0.5%)
7	p	1.13	0/572	1.12	4/762 (0.5%)
All	All	0.59	1/57169 (0.0%)	0.93	64/82911 (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
4	R	0	1
4	b	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	13	LYS	CA-C	6.37	1.57	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	84	DG	C2'-C3'-O3'	8.60	124.40	111.50
5	c	84	DG	C2'-C3'-O3'	8.54	124.31	111.50
5	c	63	DG	C2'-C3'-O3'	-8.18	99.24	111.50
2	V	50	ILE	N-CA-C	7.55	118.32	110.62
6	J	78	DA	C2'-C3'-O3'	7.51	122.76	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	R	51	ASP	Peptide

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Mol	Chain	Res	Type	Group
4	b	31	ARG	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	856	11	0
1	E	816	0	856	11	0
1	K	825	0	869	11	0
1	O	816	0	856	11	0
1	U	816	0	856	10	0
1	Y	816	0	856	14	0
1	e	825	0	869	17	0
1	i	816	0	856	10	0
2	B	638	0	676	10	0
2	F	673	0	722	4	0
2	L	638	0	676	11	0
2	P	638	0	676	7	0
2	V	638	0	676	8	0
2	Z	673	0	722	14	0
2	f	638	0	676	12	0
2	j	638	0	676	9	0
3	C	826	0	886	7	0
3	G	873	0	941	12	0
3	M	821	0	881	9	0
3	Q	810	0	866	8	0
3	W	826	0	886	9	0
3	a	873	0	941	15	0
3	g	821	0	881	12	0
3	k	810	0	866	10	0
4	D	784	0	823	9	0
4	H	784	0	823	9	0
4	N	775	0	810	4	0
4	R	775	0	810	9	0
4	X	788	0	826	12	0
4	b	788	0	826	15	0
4	h	775	0	810	10	0
4	l	775	0	810	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	3462	0	1901	30	0
5	S	3462	0	1901	22	0
5	c	3462	0	1901	33	0
5	m	3462	0	1901	18	0
6	J	3461	0	1902	22	0
6	T	3461	0	1902	11	0
6	d	3461	0	1902	16	0
6	n	3461	0	1902	10	0
7	o	583	0	608	14	0
7	p	566	0	598	13	0
8	C	1	0	0	0	0
8	G	1	0	0	0	0
8	I	8	0	0	0	0
8	J	4	0	0	0	0
8	O	2	0	0	0	0
8	S	1	0	0	0	0
8	T	3	0	0	0	0
8	W	1	0	0	0	0
8	Y	1	0	0	0	0
8	a	2	0	0	0	0
8	c	7	0	0	0	0
8	d	8	0	0	0	0
8	i	1	0	0	0	0
8	j	1	0	0	0	0
8	m	2	0	0	0	0
8	n	2	0	0	0	0
8	o	1	0	0	0	0
8	p	1	0	0	0	0
9	I	1	0	0	0	0
9	T	3	0	0	0	0
9	c	1	0	0	0	0
9	d	1	0	0	0	0
All	All	53518	0	42478	409	0

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 4.

The worst 5 of 409 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)
4:b:49:HIS:HB3	4:b:52:THR:HG23	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:100:LEU:HD11	2:f:58:LEU:HD13	1.63	0.80
4:X:95:GLN:NE2	4:X:111:VAL:HG13	1.97	0.80
1:e:60:LEU:HD13	1:e:93:GLN:HE21	1.49	0.77
4:h:76:GLU:OE2	4:h:79:ARG:NH1	2.16	0.77

There are no symmetry-related clashes.

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	97/138 (70%)	95 (98%)	2 (2%)	0	100	100
1	E	97/138 (70%)	89 (92%)	8 (8%)	0	100	100
1	K	98/138 (71%)	86 (88%)	9 (9%)	3 (3%)	3	18
1	O	97/138 (70%)	88 (91%)	8 (8%)	1 (1%)	12	40
1	U	97/138 (70%)	92 (95%)	5 (5%)	0	100	100
1	Y	97/138 (70%)	92 (95%)	3 (3%)	2 (2%)	5	24
1	e	98/138 (71%)	92 (94%)	5 (5%)	1 (1%)	12	40
1	i	97/138 (70%)	83 (86%)	12 (12%)	2 (2%)	5	24
2	B	78/105 (74%)	74 (95%)	4 (5%)	0	100	100
2	F	82/105 (78%)	76 (93%)	6 (7%)	0	100	100
2	L	78/105 (74%)	72 (92%)	6 (8%)	0	100	100
2	P	78/105 (74%)	66 (85%)	10 (13%)	2 (3%)	4	21
2	V	78/105 (74%)	75 (96%)	3 (4%)	0	100	100
2	Z	82/105 (78%)	78 (95%)	4 (5%)	0	100	100
2	f	78/105 (74%)	70 (90%)	8 (10%)	0	100	100
2	j	78/105 (74%)	70 (90%)	6 (8%)	2 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	105/132 (80%)	99 (94%)	6 (6%)	0	100	100
3	G	112/132 (85%)	102 (91%)	9 (8%)	1 (1%)	14	42
3	M	104/132 (79%)	90 (86%)	13 (12%)	1 (1%)	12	40
3	Q	103/132 (78%)	97 (94%)	6 (6%)	0	100	100
3	W	105/132 (80%)	100 (95%)	5 (5%)	0	100	100
3	a	112/132 (85%)	97 (87%)	12 (11%)	3 (3%)	4	20
3	g	104/132 (79%)	97 (93%)	7 (7%)	0	100	100
3	k	103/132 (78%)	97 (94%)	5 (5%)	1 (1%)	12	40
4	D	97/128 (76%)	89 (92%)	7 (7%)	1 (1%)	12	40
4	H	97/128 (76%)	86 (89%)	7 (7%)	4 (4%)	2	15
4	N	96/128 (75%)	85 (88%)	11 (12%)	0	100	100
4	R	96/128 (75%)	88 (92%)	6 (6%)	2 (2%)	5	24
4	X	98/128 (77%)	89 (91%)	7 (7%)	2 (2%)	6	25
4	b	98/128 (77%)	84 (86%)	13 (13%)	1 (1%)	12	40
4	h	96/128 (75%)	88 (92%)	8 (8%)	0	100	100
4	l	96/128 (75%)	84 (88%)	10 (10%)	2 (2%)	5	24
7	o	74/195 (38%)	64 (86%)	8 (11%)	2 (3%)	4	20
7	p	72/195 (37%)	66 (92%)	3 (4%)	3 (4%)	2	14
All	All	3178/4414 (72%)	2900 (91%)	242 (8%)	36 (1%)	11	38

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	14	ALA
4	H	32	SER
4	X	104	GLY
3	a	13	LYS
3	a	14	ALA

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	86/112 (77%)	85 (99%)	1 (1%)	63	72
1	E	86/112 (77%)	81 (94%)	5 (6%)	18	45
1	K	87/112 (78%)	82 (94%)	5 (6%)	18	45
1	O	86/112 (77%)	81 (94%)	5 (6%)	18	45
1	U	86/112 (77%)	84 (98%)	2 (2%)	44	63
1	Y	86/112 (77%)	80 (93%)	6 (7%)	14	40
1	e	87/112 (78%)	83 (95%)	4 (5%)	24	50
1	i	86/112 (77%)	83 (96%)	3 (4%)	32	56
2	B	65/80 (81%)	63 (97%)	2 (3%)	35	59
2	F	69/80 (86%)	64 (93%)	5 (7%)	13	39
2	L	65/80 (81%)	64 (98%)	1 (2%)	57	69
2	P	65/80 (81%)	62 (95%)	3 (5%)	24	50
2	V	65/80 (81%)	63 (97%)	2 (3%)	35	59
2	Z	69/80 (86%)	65 (94%)	4 (6%)	18	45
2	f	65/80 (81%)	64 (98%)	1 (2%)	57	69
2	j	65/80 (81%)	63 (97%)	2 (3%)	35	59
3	C	85/101 (84%)	77 (91%)	8 (9%)	8	29
3	G	88/101 (87%)	79 (90%)	9 (10%)	7	25
3	M	85/101 (84%)	81 (95%)	4 (5%)	23	50
3	Q	83/101 (82%)	79 (95%)	4 (5%)	23	50
3	W	85/101 (84%)	79 (93%)	6 (7%)	13	39
3	a	88/101 (87%)	80 (91%)	8 (9%)	9	30
3	g	85/101 (84%)	82 (96%)	3 (4%)	32	56
3	k	83/101 (82%)	78 (94%)	5 (6%)	17	43
4	D	85/106 (80%)	73 (86%)	12 (14%)	3	13
4	H	85/106 (80%)	75 (88%)	10 (12%)	5	20
4	N	84/106 (79%)	79 (94%)	5 (6%)	17	43
4	R	84/106 (79%)	78 (93%)	6 (7%)	13	39
4	X	85/106 (80%)	79 (93%)	6 (7%)	13	39
4	b	85/106 (80%)	79 (93%)	6 (7%)	13	39
4	h	84/106 (79%)	78 (93%)	6 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	l	84/106 (79%)	77 (92%)	7 (8%)	10	35
7	o	63/158 (40%)	49 (78%)	14 (22%)	1	3
7	p	61/158 (39%)	53 (87%)	8 (13%)	4	16
All	All	2700/3508 (77%)	2522 (93%)	178 (7%)	15	41

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	73	ASN
2	j	91	LYS
4	b	46	LYS
3	g	81	ARG
4	l	32	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	W	31	HIS
4	l	95	GLN
2	Z	64	ASN
4	l	84	ASN
7	p	41	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 53 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	99/138 (71%)	-0.89	0 100 100	79, 108, 157, 189	0
1	E	99/138 (71%)	-1.00	0 100 100	84, 109, 153, 193	0
1	K	100/138 (72%)	-0.83	0 100 100	131, 173, 218, 250	0
1	O	99/138 (71%)	-0.79	0 100 100	118, 170, 224, 260	0
1	U	99/138 (71%)	-0.83	0 100 100	78, 107, 154, 203	0
1	Y	99/138 (71%)	-0.94	0 100 100	81, 110, 151, 194	0
1	e	100/138 (72%)	-0.85	0 100 100	133, 180, 228, 269	0
1	i	99/138 (71%)	-0.85	0 100 100	130, 170, 218, 246	0
2	B	80/105 (76%)	-0.89	0 100 100	84, 108, 136, 192	0
2	F	84/105 (80%)	-0.91	0 100 100	87, 109, 162, 192	0
2	L	80/105 (76%)	-0.86	0 100 100	133, 169, 216, 236	0
2	P	80/105 (76%)	-0.95	0 100 100	120, 156, 198, 206	0
2	V	80/105 (76%)	-0.85	0 100 100	81, 106, 134, 185	0
2	Z	84/105 (80%)	-0.96	0 100 100	88, 110, 160, 201	0
2	f	80/105 (76%)	-0.81	0 100 100	141, 176, 231, 244	0
2	j	80/105 (76%)	-0.82	0 100 100	125, 166, 198, 212	0
3	C	107/132 (81%)	-0.75	0 100 100	92, 115, 162, 200	0
3	G	114/132 (86%)	-0.73	0 100 100	87, 117, 195, 228	0
3	M	106/132 (80%)	-0.73	0 100 100	137, 172, 206, 250	0
3	Q	105/132 (79%)	-0.85	0 100 100	136, 178, 213, 231	0
3	W	107/132 (81%)	-0.78	0 100 100	90, 110, 163, 197	0
3	a	114/132 (86%)	-0.66	0 100 100	87, 112, 197, 240	0
3	g	106/132 (80%)	-0.75	0 100 100	137, 178, 208, 233	0
3	k	105/132 (79%)	-0.87	0 100 100	139, 187, 218, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	D	99/128 (77%)	-0.85	0	100 100	94, 117, 177, 229 0
4	H	99/128 (77%)	-0.81	0	100 100	93, 117, 191, 225 0
4	N	98/128 (76%)	-0.87	0	100 100	122, 176, 214, 235 0
4	R	98/128 (76%)	-0.93	0	100 100	126, 167, 222, 258 0
4	X	100/128 (78%)	-0.93	0	100 100	91, 114, 191, 247 0
4	b	100/128 (78%)	-0.79	0	100 100	91, 114, 197, 256 0
4	h	98/128 (76%)	-0.88	0	100 100	133, 176, 214, 239 0
4	l	98/128 (76%)	-0.88	0	100 100	139, 181, 235, 261 0
5	I	169/169 (100%)	-1.20	0	100 100	121, 160, 275, 354 0
5	S	169/169 (100%)	-1.03	0	100 100	170, 217, 295, 343 0
5	c	169/169 (100%)	-1.18	0	100 100	121, 156, 271, 324 0
5	m	169/169 (100%)	-0.97	0	100 100	169, 226, 287, 362 0
6	J	169/169 (100%)	-1.22	0	100 100	119, 162, 262, 356 0
6	T	169/169 (100%)	-1.04	0	100 100	165, 221, 295, 341 0
6	d	169/169 (100%)	-1.18	0	100 100	117, 159, 270, 370 0
6	n	169/169 (100%)	-1.00	0	100 100	167, 224, 294, 317 0
7	o	76/195 (38%)	-0.64	0	100 100	188, 239, 263, 285 1 (1%)
7	p	74/195 (37%)	-0.53	0	100 100	179, 237, 264, 273 1 (1%)
All	All	4598/5766 (79%)	-0.91	0	100 100	78, 164, 252, 370 2 (0%)

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CA	d	106	1/1	0.65	0.10	157,157,157,157	0
9	K	T	105	1/1	0.72	0.16	172,172,172,172	0
8	CA	T	103	1/1	0.76	0.06	174,174,174,174	0
8	CA	I	105	1/1	0.77	0.10	163,163,163,163	0
8	CA	m	102	1/1	0.79	0.05	185,185,185,185	0
8	CA	p	201	1/1	0.85	0.07	155,155,155,155	0
8	CA	G	201	1/1	0.86	0.10	164,164,164,164	0
9	K	d	109	1/1	0.86	0.13	161,161,161,161	0
9	K	I	109	1/1	0.87	0.09	141,141,141,141	0
8	CA	n	102	1/1	0.87	0.05	166,166,166,166	0
8	CA	W	201	1/1	0.87	0.08	146,146,146,146	0
8	CA	d	104	1/1	0.88	0.06	160,160,160,160	0
8	CA	d	108	1/1	0.88	0.05	162,162,162,162	0
8	CA	d	107	1/1	0.89	0.06	152,152,152,152	0
9	K	T	104	1/1	0.89	0.08	157,157,157,157	0
8	CA	o	201	1/1	0.90	0.06	157,157,157,157	0
8	CA	I	107	1/1	0.91	0.05	160,160,160,160	0
8	CA	i	201	1/1	0.91	0.04	170,170,170,170	0
8	CA	J	104	1/1	0.91	0.14	130,130,130,130	0
8	CA	O	202	1/1	0.91	0.03	175,175,175,175	0
8	CA	I	101	1/1	0.91	0.09	147,147,147,147	0
8	CA	c	107	1/1	0.92	0.06	149,149,149,149	0
8	CA	I	103	1/1	0.92	0.07	130,130,130,130	0
8	CA	a	201	1/1	0.92	0.09	147,147,147,147	0
9	K	T	106	1/1	0.92	0.13	153,153,153,153	0
8	CA	m	101	1/1	0.92	0.06	159,159,159,159	0
8	CA	I	104	1/1	0.93	0.08	148,148,148,148	0
8	CA	I	108	1/1	0.93	0.04	137,137,137,137	0
8	CA	c	103	1/1	0.93	0.06	135,135,135,135	0
8	CA	c	104	1/1	0.93	0.07	159,159,159,159	0
9	K	c	108	1/1	0.93	0.07	143,143,143,143	0
8	CA	J	103	1/1	0.93	0.04	158,158,158,158	0
8	CA	d	103	1/1	0.94	0.07	139,139,139,139	0
8	CA	T	102	1/1	0.94	0.09	163,163,163,163	0
8	CA	d	105	1/1	0.94	0.04	144,144,144,144	0
8	CA	J	102	1/1	0.95	0.06	165,165,165,165	0
8	CA	d	102	1/1	0.95	0.09	128,128,128,128	0
8	CA	T	101	1/1	0.95	0.03	160,160,160,160	0
8	CA	c	105	1/1	0.95	0.04	145,145,145,145	0
8	CA	j	201	1/1	0.96	0.03	156,156,156,156	0
8	CA	Y	201	1/1	0.96	0.07	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	d	101	1/1	0.96	0.07	150,150,150,150	0
8	CA	S	101	1/1	0.96	0.03	159,159,159,159	0
8	CA	a	202	1/1	0.96	0.03	157,157,157,157	0
8	CA	c	106	1/1	0.96	0.05	153,153,153,153	0
8	CA	I	106	1/1	0.97	0.03	134,134,134,134	0
8	CA	J	101	1/1	0.97	0.06	133,133,133,133	0
8	CA	n	101	1/1	0.97	0.04	150,150,150,150	0
8	CA	O	201	1/1	0.97	0.03	157,157,157,157	0
8	CA	C	201	1/1	0.97	0.03	145,145,145,145	0
8	CA	c	102	1/1	0.97	0.04	131,131,131,131	0
8	CA	I	102	1/1	0.98	0.06	117,117,117,117	0
8	CA	c	101	1/1	0.99	0.07	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.