Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 08:17 AM JST

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

This is a Full wwPDB X-ray Structure Validation 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:

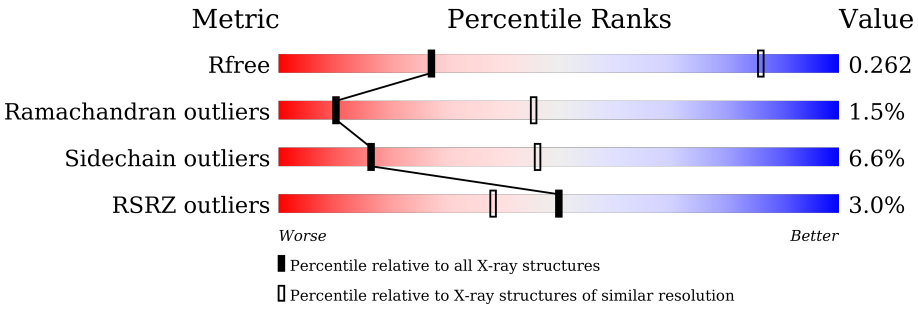
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



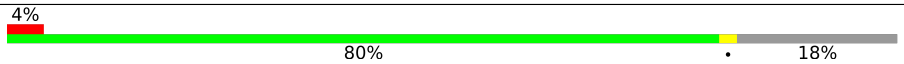
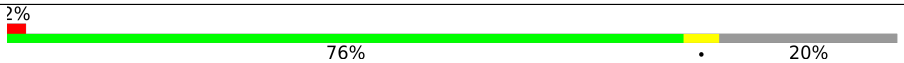
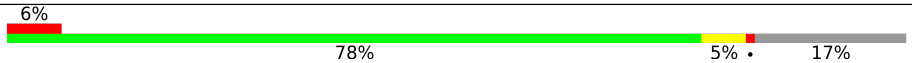
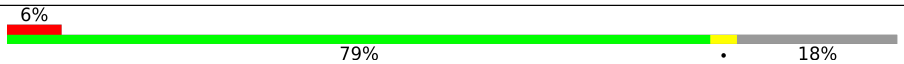
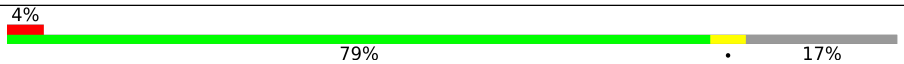
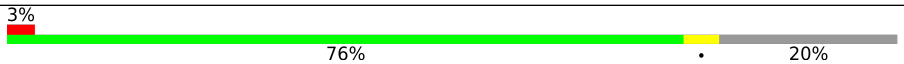
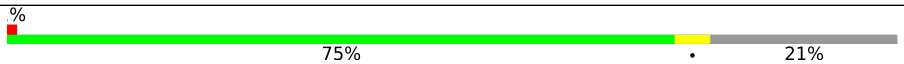
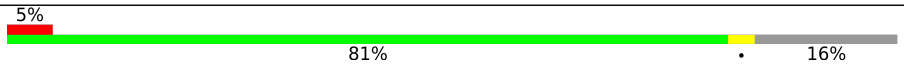
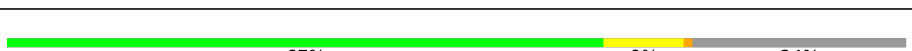
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	136	71% · 26%
1	E	136	3% 70% · 26%
1	K	136	69% · 27%
1	O	136	% 69% · 27%
1	U	136	2% 70% · 27%
1	Y	136	% 70% · 26%
1	e	136	2% 69% · 27%

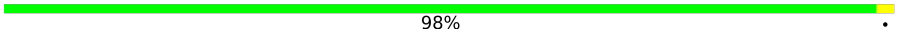
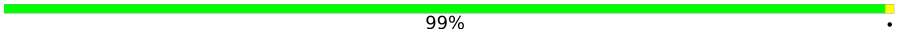
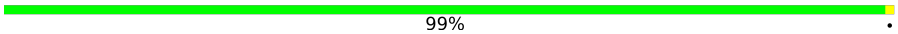
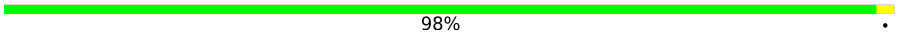
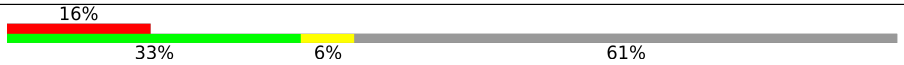
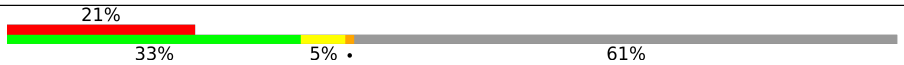
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	i	136	
2	B	103	
2	F	103	
2	L	103	
2	P	103	
2	V	103	
2	Z	103	
2	f	103	
2	j	103	
3	C	130	
3	G	130	
3	M	130	
3	Q	130	
3	W	130	
3	a	130	
3	g	130	
3	k	130	
4	D	126	
4	H	126	
4	N	126	
4	R	126	
4	X	126	
4	b	126	
4	h	126	
4	l	126	

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 53828 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.1.

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

- Molecule 2 is a protein called Histone H4.

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

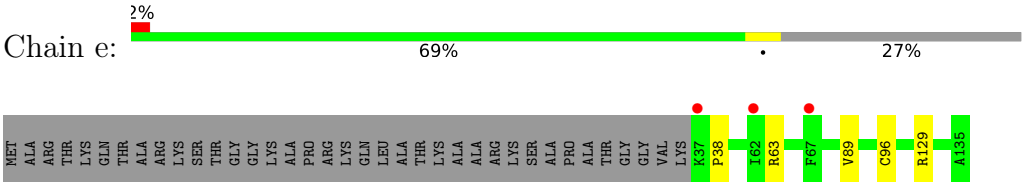
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S	75	Total	C	N	O	S	0	0	0
			575	358	108	108	1			
7	T	75	Total	C	N	O	S	0	0	0
			575	358	108	108	1			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

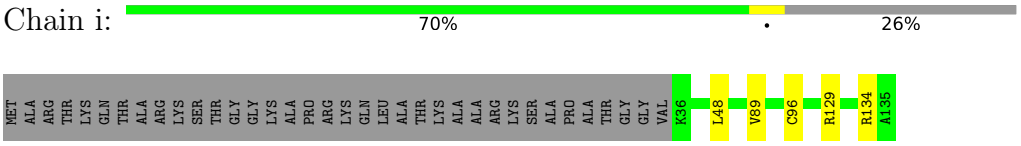
• Molecule 1: Histone H3.1

Chain e:



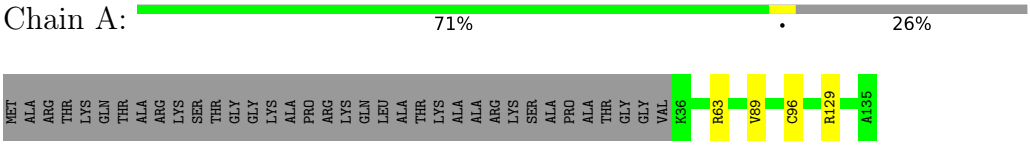
• Molecule 1: Histone H3.1

Chain i:



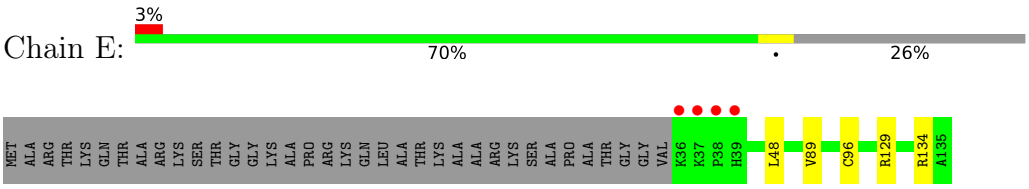
• Molecule 1: Histone H3.1

Chain A:



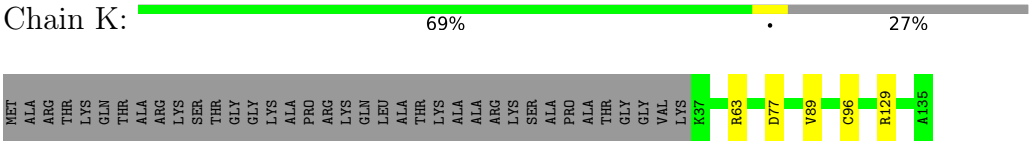
• Molecule 1: Histone H3.1

Chain E:



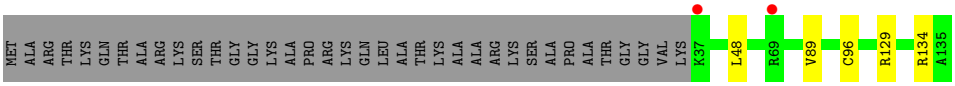
• Molecule 1: Histone H3.1

Chain K:

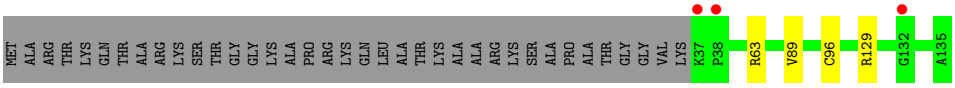


• Molecule 1: Histone H3.1

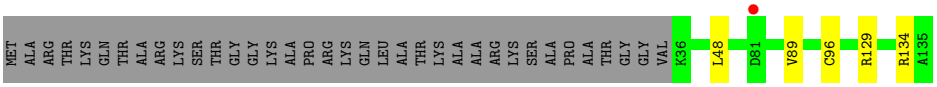
Chain O:



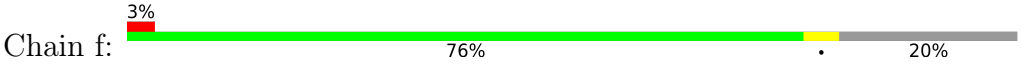
• Molecule 1: Histone H3.1



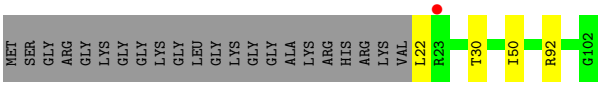
• Molecule 1: Histone H3.1



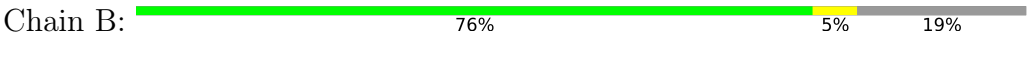
• Molecule 2: Histone H4

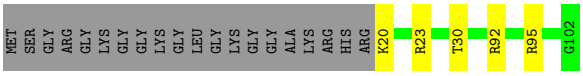


• Molecule 2: Histone H4

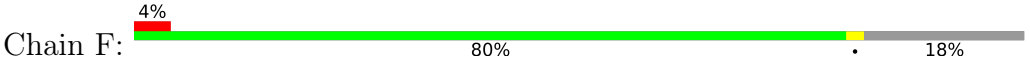


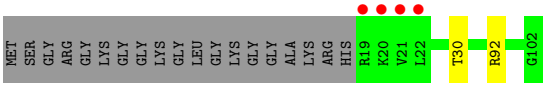
• Molecule 2: Histone H4



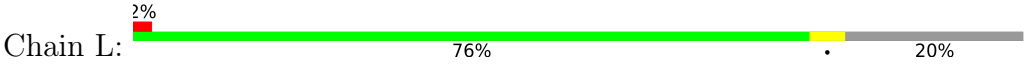


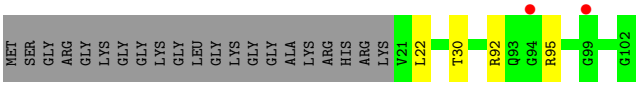
• Molecule 2: Histone H4



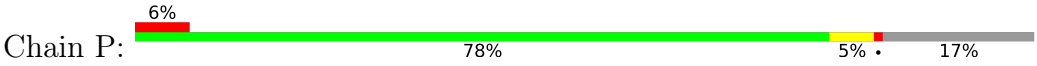


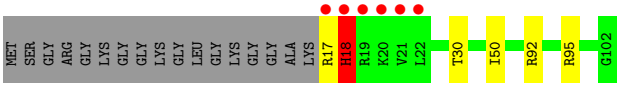
• Molecule 2: Histone H4



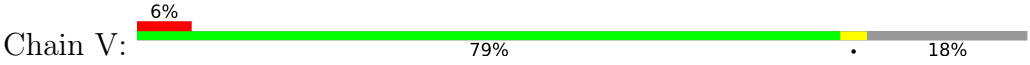


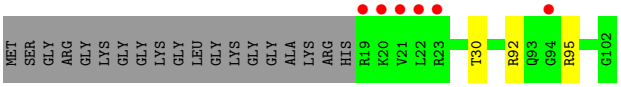
• Molecule 2: Histone H4



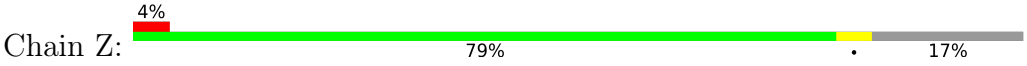


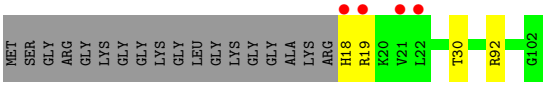
• Molecule 2: Histone H4



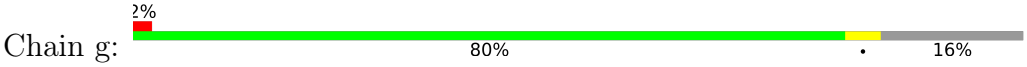


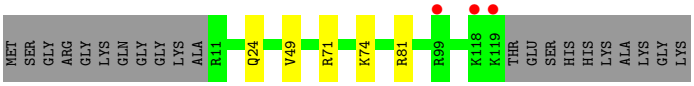
• Molecule 2: Histone H4



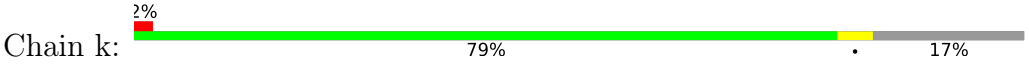


• Molecule 3: Histone H2A type 1-B/E

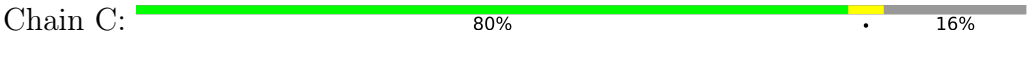


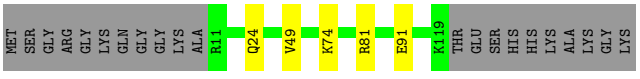


• Molecule 3: Histone H2A type 1-B/E



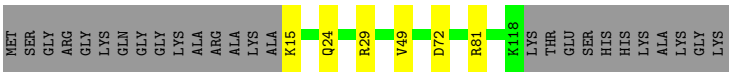
• Molecule 3: Histone H2A type 1-B/E





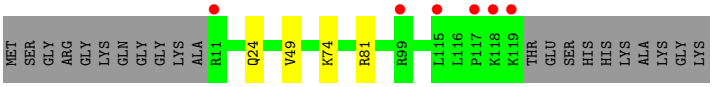
• Molecule 3: Histone H2A type 1-B/E

Chain G:



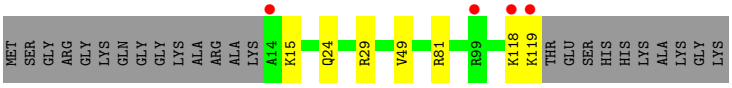
• Molecule 3: Histone H2A type 1-B/E

Chain M:



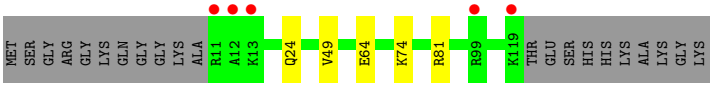
• Molecule 3: Histone H2A type 1-B/E

Chain Q:



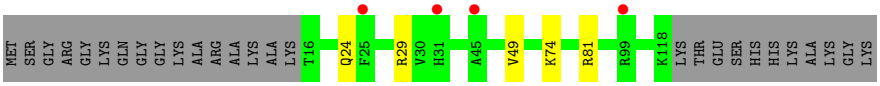
• Molecule 3: Histone H2A type 1-B/E

Chain W:



• Molecule 3: Histone H2A type 1-B/E

Chain a:



• Molecule 4: Histone H2B type 1-J

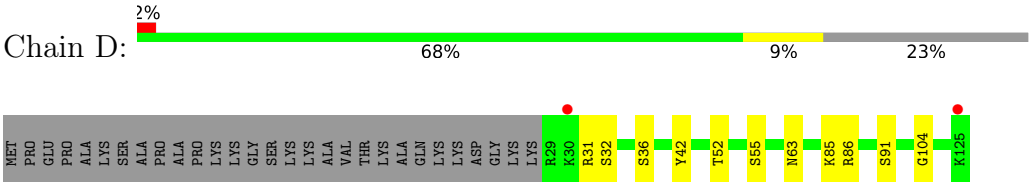
Chain h:

• Molecule 4: Histone H2B type 1-J

Chain l:

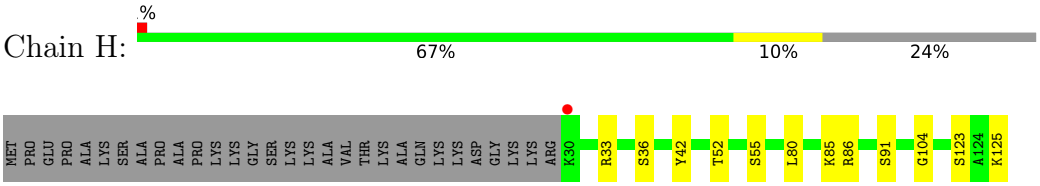
• Molecule 4: Histone H2B type 1-J

Chain D:



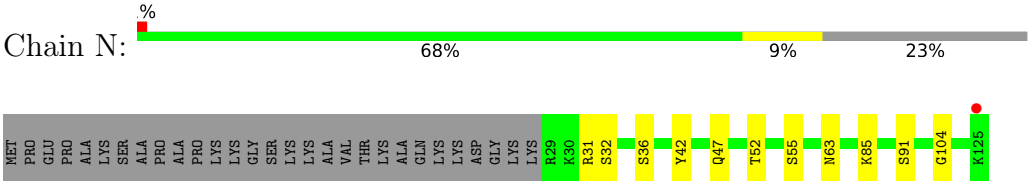
• Molecule 4: Histone H2B type 1-J

Chain H:



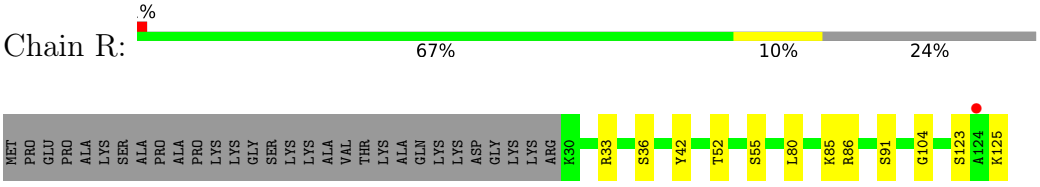
• Molecule 4: Histone H2B type 1-J

Chain N:



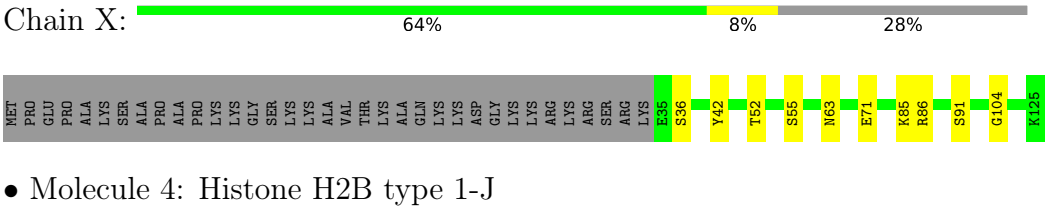
• Molecule 4: Histone H2B type 1-J

Chain R:



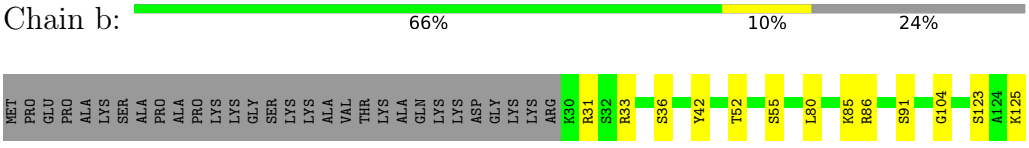
• Molecule 4: Histone H2B type 1-J

Chain X:



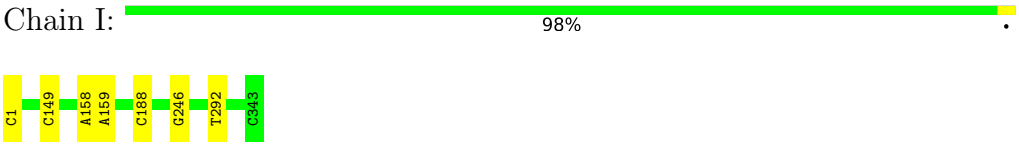
• Molecule 4: Histone H2B type 1-J

Chain b:



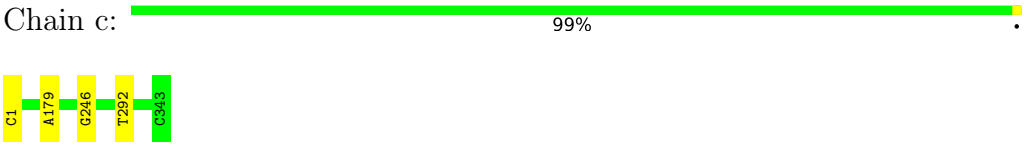
• Molecule 5: DNA (343-MER)

Chain I:



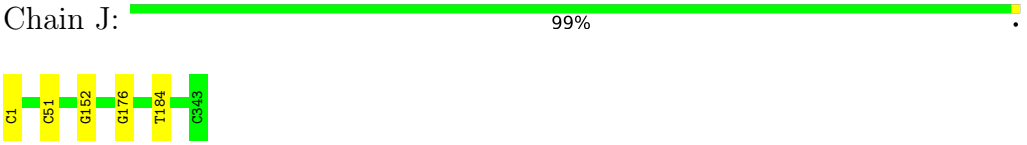
• Molecule 5: DNA (343-MER)

Chain c:



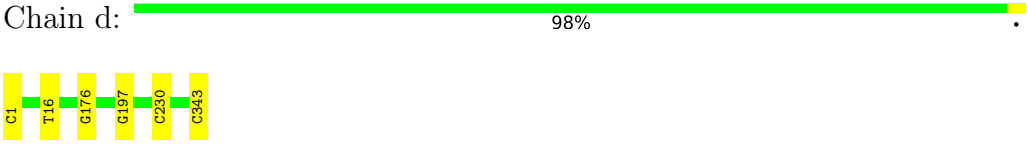
• Molecule 6: DNA (343-MER)

Chain J:



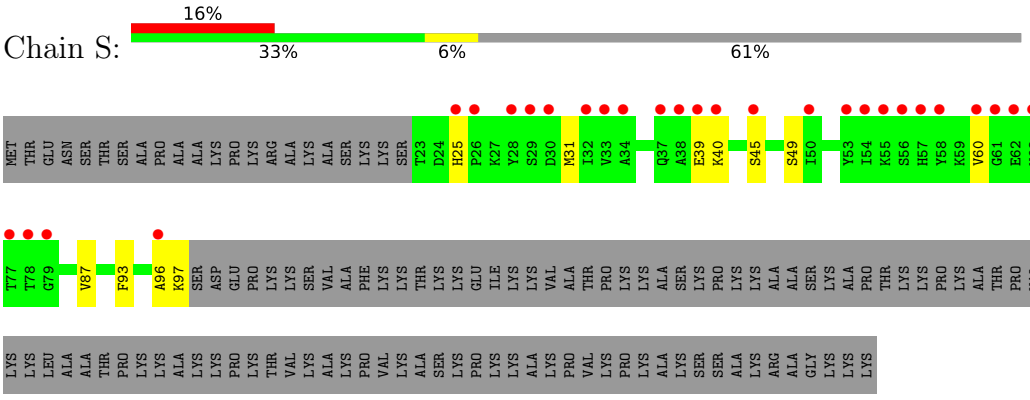
• Molecule 6: DNA (343-MER)

Chain d:



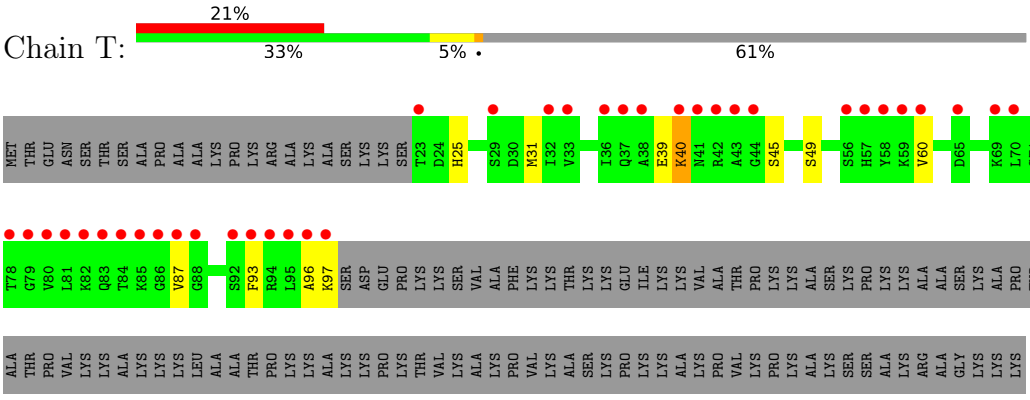
• Molecule 7: Histone H1.0

Chain S:



• Molecule 7: Histone H1.0

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.75Å 205.90Å 237.68Å 90.00° 97.19° 90.00°	Depositor
Resolution (Å)	49.35 – 3.89 49.30 – 3.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.35-3.89) 99.4 (49.30-3.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.199 , 0.267 0.202 , 0.262	Depositor DCC
R_{free} test set	1885 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	185.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 165.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53828	wwPDB-VP
Average B, all atoms (Å^2)	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.67	0/837	0.81	0/1120
1	E	0.67	0/837	0.82	0/1120
1	K	0.66	0/828	0.81	0/1109
1	O	0.65	0/828	0.81	0/1109
1	U	0.67	0/828	0.82	0/1109
1	Y	0.66	0/837	0.82	0/1120
1	e	0.66	0/828	0.79	0/1109
1	i	0.67	0/837	0.82	0/1120
2	B	0.68	0/669	0.85	0/894
2	F	0.69	0/680	0.87	0/908
2	L	0.68	0/660	0.85	0/883
2	P	0.69	0/702	0.84	0/937
2	V	0.68	0/680	0.86	0/908
2	Z	0.67	0/691	0.85	0/923
2	f	0.68	0/660	0.83	0/883
2	j	0.68	0/653	0.84	0/873
3	C	0.70	0/854	0.81	0/1150
3	G	0.68	0/815	0.77	0/1100
3	M	0.69	0/854	0.81	0/1150
3	Q	0.67	0/829	0.80	0/1118
3	W	0.69	0/854	0.80	0/1150
3	a	0.68	0/806	0.77	0/1089
3	g	0.69	0/854	0.81	0/1150
3	k	0.67	0/845	0.77	0/1139
4	D	0.70	0/777	0.80	0/1040
4	H	0.68	0/766	0.79	0/1026
4	N	0.71	0/777	0.79	0/1040
4	R	0.69	0/766	0.79	0/1026
4	X	0.70	0/720	0.79	0/968
4	b	0.71	0/766	0.80	0/1026
4	h	0.77	0/766	1.20	4/1026 (0.4%)
4	l	0.70	0/766	0.78	0/1026
5	I	0.39	2/7890 (0.0%)	0.83	5/12165 (0.0%)
5	c	0.38	1/7890 (0.0%)	0.81	3/12165 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	J	0.40	1/7888 (0.0%)	0.83	5/12180 (0.0%)
6	d	0.38	1/7888 (0.0%)	0.81	5/12180 (0.0%)
7	S	0.75	0/581	0.82	0/775
7	T	0.73	0/581	0.81	0/775
All	All	0.54	5/57588 (0.0%)	0.82	22/83589 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1	DC	OP3-P	-10.56	1.48	1.61
5	c	1	DC	OP3-P	-10.51	1.48	1.61
6	d	1	DC	OP3-P	-10.31	1.48	1.61
5	I	1	DC	OP3-P	-9.59	1.49	1.61
5	I	149	DC	O3'-P	-5.20	1.54	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	31	ARG	NE-CZ-NH2	-20.69	109.95	120.30
4	h	31	ARG	NE-CZ-NH1	17.92	129.26	120.30
6	J	176	DG	C1'-O4'-C4'	-8.98	101.12	110.10
5	I	158	DA	C1'-O4'-C4'	-7.55	102.55	110.10
5	I	159	DA	C1'-O4'-C4'	-7.25	102.86	110.10
6	J	184	DT	C1'-O4'-C4'	-6.23	103.87	110.10
4	h	31	ARG	CG-CD-NE	6.20	124.81	111.80
6	J	152	DG	C1'-O4'-C4'	-5.84	104.26	110.10
4	h	31	ARG	CD-NE-CZ	-5.64	115.70	123.60
6	J	176	DG	N9-C1'-C2'	5.55	123.15	112.60
6	d	176	DG	C1'-O4'-C4'	-5.38	104.72	110.10
5	I	246	DG	C1'-O4'-C4'	-5.37	104.73	110.10
6	d	343	DC	C1'-O4'-C4'	-5.34	104.76	110.10
5	c	246	DG	C1'-O4'-C4'	-5.32	104.78	110.10
6	d	197	DG	C1'-O4'-C4'	-5.29	104.81	110.10
5	c	292	DT	C1'-O4'-C4'	-5.26	104.84	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	51	DC	C1'-O4'-C4'	-5.24	104.86	110.10
5	c	179	DA	C1'-O4'-C4'	-5.20	104.90	110.10
5	I	292	DT	C1'-O4'-C4'	-5.18	104.92	110.10
5	I	188	DC	C1'-O4'-C4'	-5.16	104.94	110.10
6	d	230	DC	C1'-O4'-C4'	-5.04	105.06	110.10
6	d	16	DT	C1'-O4'-C4'	-5.03	105.07	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	18	HIS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	98/136 (72%)	83 (85%)	13 (13%)	2 (2%)	7 40
1	E	98/136 (72%)	84 (86%)	12 (12%)	2 (2%)	7 40
1	K	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)	7 39
1	O	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)	7 39
1	U	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)	7 39
1	Y	98/136 (72%)	84 (86%)	12 (12%)	2 (2%)	7 40
1	e	97/136 (71%)	82 (84%)	12 (12%)	3 (3%)	4 32
1	i	98/136 (72%)	83 (85%)	13 (13%)	2 (2%)	7 40
2	B	81/103 (79%)	62 (76%)	19 (24%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	82/103 (80%)	65 (79%)	17 (21%)	0	100	100
2	L	80/103 (78%)	64 (80%)	16 (20%)	0	100	100
2	P	84/103 (82%)	65 (77%)	18 (21%)	1 (1%)	13	49
2	V	82/103 (80%)	64 (78%)	18 (22%)	0	100	100
2	Z	83/103 (81%)	64 (77%)	19 (23%)	0	100	100
2	f	80/103 (78%)	63 (79%)	17 (21%)	0	100	100
2	j	79/103 (77%)	61 (77%)	18 (23%)	0	100	100
3	C	107/130 (82%)	93 (87%)	13 (12%)	1 (1%)	17	54
3	G	102/130 (78%)	90 (88%)	11 (11%)	1 (1%)	15	52
3	M	107/130 (82%)	95 (89%)	11 (10%)	1 (1%)	17	54
3	Q	104/130 (80%)	92 (88%)	11 (11%)	1 (1%)	15	52
3	W	107/130 (82%)	94 (88%)	12 (11%)	1 (1%)	17	54
3	a	101/130 (78%)	89 (88%)	11 (11%)	1 (1%)	15	52
3	g	107/130 (82%)	94 (88%)	12 (11%)	1 (1%)	17	54
3	k	106/130 (82%)	93 (88%)	12 (11%)	1 (1%)	17	54
4	D	95/126 (75%)	73 (77%)	21 (22%)	1 (1%)	14	51
4	H	94/126 (75%)	71 (76%)	21 (22%)	2 (2%)	7	39
4	N	95/126 (75%)	73 (77%)	21 (22%)	1 (1%)	14	51
4	R	94/126 (75%)	71 (76%)	21 (22%)	2 (2%)	7	39
4	X	89/126 (71%)	70 (79%)	18 (20%)	1 (1%)	14	51
4	b	94/126 (75%)	70 (74%)	22 (23%)	2 (2%)	7	39
4	h	94/126 (75%)	72 (77%)	20 (21%)	2 (2%)	7	39
4	l	94/126 (75%)	70 (74%)	22 (23%)	2 (2%)	7	39
7	S	73/194 (38%)	59 (81%)	10 (14%)	4 (6%)	2	22
7	T	73/194 (38%)	59 (81%)	10 (14%)	4 (6%)	2	22
All	All	3167/4348 (73%)	2601 (82%)	519 (16%)	47 (2%)	10	45

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	l	33	ARG
4	H	33	ARG
7	S	87	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	T	87	VAL
2	P	18	HIS
4	R	33	ARG
4	b	33	ARG
4	h	104	GLY
4	l	104	GLY
4	D	104	GLY
4	H	104	GLY
7	T	39	GLU
7	T	40	LYS
4	N	104	GLY
4	R	104	GLY
4	X	104	GLY
4	b	104	GLY
7	S	39	GLU
7	S	40	LYS
1	A	96	CYS
1	E	96	CYS
1	e	96	CYS
1	i	96	CYS
1	K	96	CYS
1	O	96	CYS
1	U	96	CYS
1	Y	96	CYS
1	e	38	PRO
4	h	31	ARG
7	S	96	ALA
7	T	96	ALA
1	i	89	VAL
1	e	89	VAL
3	g	49	VAL
3	k	49	VAL
1	A	89	VAL
3	C	49	VAL
1	E	89	VAL
3	G	49	VAL
1	K	89	VAL
3	M	49	VAL
1	O	89	VAL
3	Q	49	VAL
1	U	89	VAL
3	W	49	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	89	VAL
3	a	49	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/111 (78%)	85 (98%)	2 (2%)	50	71
1	E	87/111 (78%)	84 (97%)	3 (3%)	37	62
1	K	86/111 (78%)	84 (98%)	2 (2%)	50	71
1	O	86/111 (78%)	83 (96%)	3 (4%)	36	62
1	U	86/111 (78%)	84 (98%)	2 (2%)	50	71
1	Y	87/111 (78%)	84 (97%)	3 (3%)	37	62
1	e	86/111 (78%)	84 (98%)	2 (2%)	50	71
1	i	87/111 (78%)	84 (97%)	3 (3%)	37	62
2	B	68/79 (86%)	63 (93%)	5 (7%)	13	43
2	F	69/79 (87%)	67 (97%)	2 (3%)	42	65
2	L	67/79 (85%)	63 (94%)	4 (6%)	19	49
2	P	71/79 (90%)	65 (92%)	6 (8%)	10	39
2	V	69/79 (87%)	66 (96%)	3 (4%)	29	57
2	Z	70/79 (89%)	66 (94%)	4 (6%)	20	50
2	f	67/79 (85%)	63 (94%)	4 (6%)	19	49
2	j	66/79 (84%)	63 (96%)	3 (4%)	27	56
3	C	86/100 (86%)	82 (95%)	4 (5%)	26	55
3	G	83/100 (83%)	79 (95%)	4 (5%)	25	54
3	M	86/100 (86%)	83 (96%)	3 (4%)	36	62
3	Q	84/100 (84%)	78 (93%)	6 (7%)	14	44
3	W	86/100 (86%)	83 (96%)	3 (4%)	36	62
3	a	82/100 (82%)	78 (95%)	4 (5%)	25	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	g	86/100 (86%)	82 (95%)	4 (5%)	26 55
3	k	85/100 (85%)	81 (95%)	4 (5%)	26 55
4	D	83/105 (79%)	73 (88%)	10 (12%)	5 25
4	H	82/105 (78%)	72 (88%)	10 (12%)	5 24
4	N	83/105 (79%)	73 (88%)	10 (12%)	5 25
4	R	82/105 (78%)	72 (88%)	10 (12%)	5 24
4	X	77/105 (73%)	68 (88%)	9 (12%)	5 26
4	b	82/105 (78%)	71 (87%)	11 (13%)	4 22
4	h	82/105 (78%)	72 (88%)	10 (12%)	5 24
4	l	82/105 (78%)	71 (87%)	11 (13%)	4 22
7	S	62/158 (39%)	55 (89%)	7 (11%)	6 27
7	T	62/158 (39%)	54 (87%)	8 (13%)	4 23
All	All	2694/3476 (78%)	2515 (93%)	179 (7%)	16 46

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	63	ARG
1	e	129	ARG
2	f	30	THR
2	f	50	ILE
2	f	92	ARG
2	f	95	ARG
3	g	24	GLN
3	g	71	ARG
3	g	74	LYS
3	g	81	ARG
4	h	32	SER
4	h	36	SER
4	h	42	TYR
4	h	52	THR
4	h	55	SER
4	h	63	ASN
4	h	71	GLU
4	h	85	LYS
4	h	86	ARG
4	h	91	SER
1	i	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	i	129	ARG
1	i	134	ARG
2	j	30	THR
2	j	50	ILE
2	j	92	ARG
3	k	11	ARG
3	k	15	LYS
3	k	24	GLN
3	k	81	ARG
4	l	31	ARG
4	l	36	SER
4	l	42	TYR
4	l	52	THR
4	l	55	SER
4	l	80	LEU
4	l	85	LYS
4	l	86	ARG
4	l	91	SER
4	l	123	SER
4	l	125	LYS
1	A	63	ARG
1	A	129	ARG
2	B	20	LYS
2	B	23	ARG
2	B	30	THR
2	B	92	ARG
2	B	95	ARG
3	C	24	GLN
3	C	74	LYS
3	C	81	ARG
3	C	91	GLU
4	D	31	ARG
4	D	32	SER
4	D	36	SER
4	D	42	TYR
4	D	52	THR
4	D	55	SER
4	D	63	ASN
4	D	85	LYS
4	D	86	ARG
4	D	91	SER
1	E	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	129	ARG
1	E	134	ARG
2	F	30	THR
2	F	92	ARG
3	G	15	LYS
3	G	24	GLN
3	G	29	ARG
3	G	81	ARG
4	H	36	SER
4	H	42	TYR
4	H	52	THR
4	H	55	SER
4	H	80	LEU
4	H	85	LYS
4	H	86	ARG
4	H	91	SER
4	H	123	SER
4	H	125	LYS
7	S	25	HIS
7	S	31	MET
7	S	45	SER
7	S	49	SER
7	S	60	VAL
7	S	93	PHE
7	S	97	LYS
7	T	25	HIS
7	T	31	MET
7	T	40	LYS
7	T	45	SER
7	T	49	SER
7	T	60	VAL
7	T	93	PHE
7	T	97	LYS
1	K	63	ARG
1	K	129	ARG
2	L	22	LEU
2	L	30	THR
2	L	92	ARG
2	L	95	ARG
3	M	24	GLN
3	M	74	LYS
3	M	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	31	ARG
4	N	32	SER
4	N	36	SER
4	N	42	TYR
4	N	47	GLN
4	N	52	THR
4	N	55	SER
4	N	63	ASN
4	N	85	LYS
4	N	91	SER
1	O	48	LEU
1	O	129	ARG
1	O	134	ARG
2	P	17	ARG
2	P	18	HIS
2	P	30	THR
2	P	50	ILE
2	P	92	ARG
2	P	95	ARG
3	Q	15	LYS
3	Q	24	GLN
3	Q	29	ARG
3	Q	81	ARG
3	Q	118	LYS
3	Q	119	LYS
4	R	36	SER
4	R	42	TYR
4	R	52	THR
4	R	55	SER
4	R	80	LEU
4	R	85	LYS
4	R	86	ARG
4	R	91	SER
4	R	123	SER
4	R	125	LYS
1	U	63	ARG
1	U	129	ARG
2	V	30	THR
2	V	92	ARG
2	V	95	ARG
3	W	24	GLN
3	W	74	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	81	ARG
4	X	36	SER
4	X	42	TYR
4	X	52	THR
4	X	55	SER
4	X	63	ASN
4	X	71	GLU
4	X	85	LYS
4	X	86	ARG
4	X	91	SER
1	Y	48	LEU
1	Y	129	ARG
1	Y	134	ARG
2	Z	18	HIS
2	Z	19	ARG
2	Z	30	THR
2	Z	92	ARG
3	a	24	GLN
3	a	29	ARG
3	a	74	LYS
3	a	81	ARG
4	b	31	ARG
4	b	36	SER
4	b	42	TYR
4	b	52	THR
4	b	55	SER
4	b	80	LEU
4	b	85	LYS
4	b	86	ARG
4	b	91	SER
4	b	123	SER
4	b	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	g	24	GLN
4	h	47	GLN
4	h	63	ASN
4	h	67	ASN
4	h	95	GLN
1	i	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	j	64	ASN
4	l	95	GLN
3	C	24	GLN
4	D	63	ASN
4	D	67	ASN
4	D	95	GLN
1	E	76	GLN
2	F	64	ASN
4	N	49	HIS
4	N	63	ASN
4	N	67	ASN
4	N	95	GLN
1	O	76	GLN
2	P	64	ASN
3	Q	24	GLN
3	Q	38	ASN
4	R	95	GLN
4	R	109	HIS
3	W	24	GLN
4	X	47	GLN
4	X	49	HIS
4	X	63	ASN
4	X	67	ASN
4	X	95	GLN
1	Y	76	GLN
2	Z	64	ASN
3	a	24	GLN
3	a	68	ASN
4	b	95	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	100/136 (73%)	-0.45	0 100 100	122, 175, 243, 313	0
1	E	100/136 (73%)	-0.40	4 (4%) 38 30	89, 163, 240, 277	0
1	K	99/136 (72%)	-0.40	0 100 100	125, 168, 232, 344	0
1	O	99/136 (72%)	-0.16	2 (2%) 65 55	133, 192, 258, 309	0
1	U	99/136 (72%)	-0.26	3 (3%) 50 38	112, 166, 226, 290	0
1	Y	100/136 (73%)	-0.29	1 (1%) 82 75	146, 211, 270, 310	0
1	e	99/136 (72%)	-0.27	3 (3%) 50 38	122, 191, 265, 313	0
1	i	100/136 (73%)	-0.44	0 100 100	123, 173, 259, 297	0
2	B	83/103 (80%)	-0.30	0 100 100	112, 162, 226, 452	0
2	F	84/103 (81%)	-0.17	4 (4%) 30 25	112, 162, 280, 391	0
2	L	82/103 (79%)	-0.19	2 (2%) 59 48	125, 161, 208, 255	0
2	P	86/103 (83%)	0.38	6 (6%) 16 12	140, 202, 306, 364	0
2	V	84/103 (81%)	-0.04	6 (7%) 16 11	118, 159, 249, 399	0
2	Z	85/103 (82%)	-0.11	4 (4%) 31 25	143, 204, 283, 336	0
2	f	82/103 (79%)	-0.24	3 (3%) 41 32	144, 190, 231, 423	0
2	j	81/103 (78%)	-0.20	1 (1%) 79 70	116, 162, 219, 338	0
3	C	109/130 (83%)	-0.35	0 100 100	103, 167, 239, 270	0
3	G	104/130 (80%)	-0.21	0 100 100	128, 183, 243, 285	0
3	M	109/130 (83%)	-0.15	6 (5%) 25 20	162, 220, 297, 357	0
3	Q	106/130 (81%)	-0.12	4 (3%) 40 31	125, 196, 262, 323	0
3	W	109/130 (83%)	-0.14	5 (4%) 32 26	116, 185, 264, 298	0
3	a	103/130 (79%)	-0.22	4 (3%) 39 30	126, 197, 273, 365	0
3	g	109/130 (83%)	-0.18	3 (2%) 53 41	109, 175, 267, 308	0
3	k	108/130 (83%)	-0.27	2 (1%) 66 57	163, 213, 278, 360	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
4	D	97/126 (76%)	-0.25	2 (2%) 63 53	110, 169, 252, 326	0
4	H	96/126 (76%)	-0.43	1 (1%) 82 75	109, 180, 245, 282	0
4	N	97/126 (76%)	-0.40	1 (1%) 82 75	155, 220, 301, 328	0
4	R	96/126 (76%)	-0.35	1 (1%) 82 75	145, 201, 264, 298	0
4	X	91/126 (72%)	-0.35	0 100 100	125, 178, 240, 296	0
4	b	96/126 (76%)	-0.40	0 100 100	127, 209, 267, 330	0
4	h	96/126 (76%)	-0.43	0 100 100	122, 181, 250, 298	0
4	l	96/126 (76%)	-0.41	0 100 100	154, 213, 286, 318	0
5	I	343/343 (100%)	-0.97	0 100 100	151, 264, 394, 469	0
5	c	343/343 (100%)	-0.99	0 100 100	155, 266, 391, 518	0
6	J	343/343 (100%)	-0.97	0 100 100	112, 266, 386, 446	0
6	d	343/343 (100%)	-0.95	0 100 100	159, 274, 404, 479	0
7	S	75/194 (38%)	2.00	31 (41%) 0 0	234, 312, 398, 432	1 (1%)
7	T	75/194 (38%)	2.97	40 (53%) 0 0	273, 348, 409, 437	1 (1%)
All	All	4607/5720 (80%)	-0.38	139 (3%) 50 38	89, 209, 350, 518	2 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	18	HIS	13.5
7	T	86	GLY	13.1
2	P	17	ARG	11.3
7	T	96	ALA	9.9
7	S	61	GLY	9.1
7	T	85	LYS	8.5
2	F	19	ARG	8.2
2	P	21	VAL	8.0
7	T	95	LEU	7.8
7	T	42	ARG	7.7
2	P	19	ARG	7.6
1	U	37	LYS	7.5
7	T	40	LYS	7.5
7	T	83	GLN	7.5
7	S	60	VAL	7.1
2	P	20	LYS	7.1
7	S	62	GLU	7.1
7	T	77	THR	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	T	84	THR	6.7
2	P	22	LEU	6.4
7	T	41	ASN	6.0
7	T	43	ALA	6.0
7	T	59	LYS	5.9
1	U	38	PRO	5.8
7	S	54	ILE	5.8
7	T	76	VAL	5.8
7	T	57	HIS	5.6
7	T	79	GLY	5.5
7	S	55	LYS	5.4
7	T	94	ARG	5.4
7	S	37	GLN	5.3
7	S	65	ASP	5.3
7	S	32	ILE	5.3
7	S	29	SER	5.2
7	S	56	SER	5.2
7	T	60	VAL	5.2
7	S	77	THR	5.2
7	T	78	THR	5.0
1	E	36	LYS	4.8
2	Z	18	HIS	4.8
7	S	79	GLY	4.8
2	F	22	LEU	4.8
7	S	33	VAL	4.5
7	T	88	GLY	4.5
7	T	37	GLN	4.5
2	Z	22	LEU	4.4
2	V	22	LEU	4.4
7	S	38	ALA	4.3
7	T	38	ALA	4.3
7	S	40	LYS	4.3
7	T	87	VAL	4.2
7	T	72	ILE	4.1
7	T	56	SER	4.0
1	E	38	PRO	4.0
2	F	21	VAL	4.0
2	V	94	GLY	3.9
7	S	28	TYR	3.9
2	V	19	ARG	3.9
7	T	97	LYS	3.9
2	Z	19	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	W	11	ARG	3.8
7	S	78	THR	3.7
7	T	69	LYS	3.6
1	O	37	LYS	3.6
7	T	80	VAL	3.6
2	j	23	ARG	3.5
3	Q	99	ARG	3.5
7	S	45	SER	3.5
1	E	39	HIS	3.5
7	T	36	ILE	3.4
7	S	30	ASP	3.3
1	E	37	LYS	3.3
7	T	92	SER	3.3
7	S	57	HIS	3.3
7	S	58	TYR	3.2
2	V	20	LYS	3.2
7	T	58	TYR	3.2
7	S	39	GLU	3.2
3	k	31	HIS	3.2
7	S	53	TYR	3.2
2	f	21	VAL	3.1
7	T	29	SER	3.1
7	T	82	LYS	3.1
3	g	99	ARG	3.0
7	T	23	THR	3.0
3	g	119	LYS	3.0
3	k	99	ARG	3.0
7	S	64	ALA	3.0
3	a	99	ARG	3.0
4	D	30	LYS	3.0
4	D	125	LYS	3.0
7	S	96	ALA	3.0
7	S	34	ALA	2.9
3	a	31	HIS	2.9
3	W	119	LYS	2.9
3	Q	14	ALA	2.9
1	e	67	PHE	2.8
2	L	94	GLY	2.7
2	F	20	LYS	2.7
2	V	23	ARG	2.7
3	M	119	LYS	2.7
1	e	37	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	118	LYS	2.7
7	S	50	ILE	2.6
3	Q	119	LYS	2.6
7	T	32	ILE	2.6
1	e	62	ILE	2.6
3	M	117	PRO	2.6
7	S	63	ASN	2.5
2	V	21	VAL	2.5
7	T	44	GLY	2.5
7	T	65	ASP	2.5
7	T	81	LEU	2.4
3	M	118	LYS	2.4
2	Z	21	VAL	2.4
3	W	99	ARG	2.4
2	f	22	LEU	2.4
7	S	76	VAL	2.4
4	H	30	LYS	2.4
3	a	45	ALA	2.3
7	S	25	HIS	2.3
3	M	115	LEU	2.2
7	T	33	VAL	2.2
3	W	13	LYS	2.2
7	S	26	PRO	2.1
1	O	69	ARG	2.1
3	M	11	ARG	2.1
3	M	99	ARG	2.1
4	R	124	ALA	2.1
7	T	70	LEU	2.1
4	N	125	LYS	2.1
2	L	99	GLY	2.1
7	T	93	PHE	2.1
3	g	118	LYS	2.1
2	f	28	GLY	2.1
3	a	25	PHE	2.0
3	W	12	ALA	2.0
1	Y	81	ASP	2.0
1	U	132	GLY	2.0

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 monosaccharides 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.