



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 03:50 am BST

PDB ID : 1M19
Title : LIGAND BINDING ALTERS THE STRUCTURE AND DYNAMICS OF NUCLEOSOMAL DNA
Authors : Suto, R.K.; Edayathumangalam, R.S.; White, C.L.; Melander, C.; Gottesfeld, J.M.; Dervan, P.B.; Luger, K.
Deposited on : 2002-06-18
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

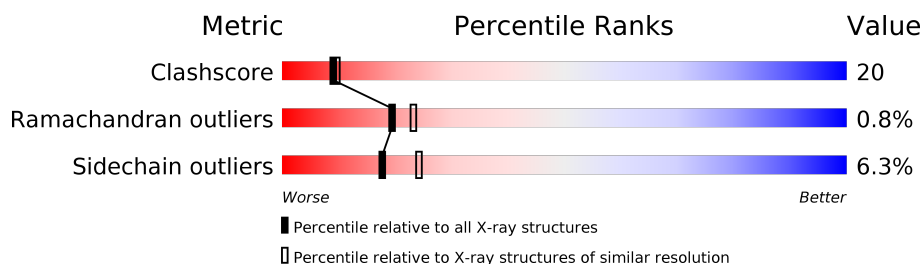
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)



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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	45% 54% .
1	J	146	47% 51% .
2	A	135	59% 10% . . 26%
2	E	135	53% 15% . . 27%
3	B	102	64% 13% . 23%
3	F	102	61% 21% . . 16%
4	C	129	67% 11% . . 17%
4	G	129	63% 15% . . 19%

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Mol	Chain	Length	Quality of chain
5	D	125	
5	H	125	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	IMT	I	1961	-	-	X	-
7	IMT	J	1901	-	-	X	-
8	PYB	I	1962	-	-	X	-
8	PYB	I	1963	-	-	X	-
8	PYB	I	1964	-	-	X	-
8	PYB	I	1967	-	-	X	-
8	PYB	I	1968	-	-	X	-
8	PYB	I	1969	-	-	X	-
8	PYB	I	2022	-	-	X	-
8	PYB	I	2023	-	-	X	-
8	PYB	I	2024	-	-	X	-
8	PYB	I	2028	-	-	X	-
8	PYB	I	2029	-	-	X	-
8	PYB	J	1902	-	-	X	-
8	PYB	J	1903	-	-	X	-
8	PYB	J	1904	-	-	X	-
8	PYB	J	1906	-	-	X	-
8	PYB	J	1907	-	-	X	-
8	PYB	J	1908	-	-	X	-
8	PYB	J	1922	-	-	X	-
8	PYB	J	1923	-	-	X	-
8	PYB	J	1924	-	-	X	-
8	PYB	J	1927	-	-	X	-
8	PYB	J	1928	-	-	X	-
8	PYB	J	1929	-	-	X	-
8	PYB	J	2002	-	-	X	-
8	PYB	J	2003	-	-	X	-
8	PYB	J	2006	-	-	X	-
8	PYB	J	2007	-	-	X	-
8	PYB	J	2008	-	-	X	-
8	PYB	J	2009	-	-	X	-
9	ABU	J	1905	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13158 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 DNA chain called Palindromic 146 Base Pair DNA Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			
1	J	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	100	Total	C	N	O	S	0	0	0
			826	521	160	142	3			
2	E	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	SER	ARG	SEE REMARK 999	UNP P02302
E	686	SER	ARG	SEE REMARK 999	UNP P02302

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
3	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

- Molecule 4 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	107	Total	C	N	O	0	0	0
			825	520	161	144			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	105	Total	C	N	O	0	0	0
			813	513	159	141			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	899	ARG	GLY	SEE REMARK 999	UNP P06897
G	1099	ARG	GLY	SEE REMARK 999	UNP P06897

- Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			
5	H	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			

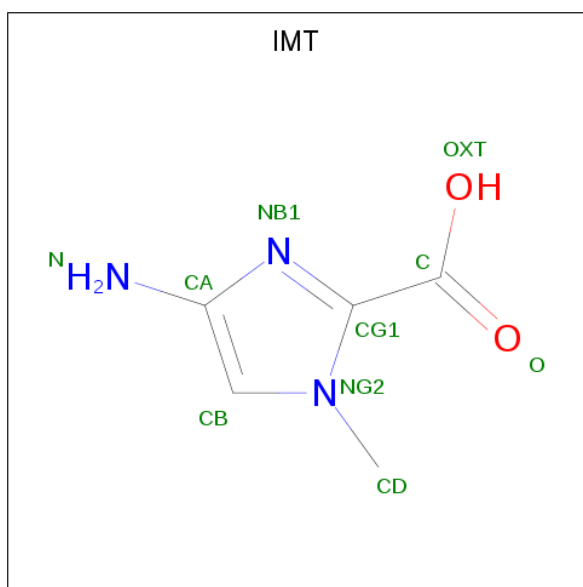
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1229	THR	SER	SEE REMARK 999	UNP P02281
H	1429	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

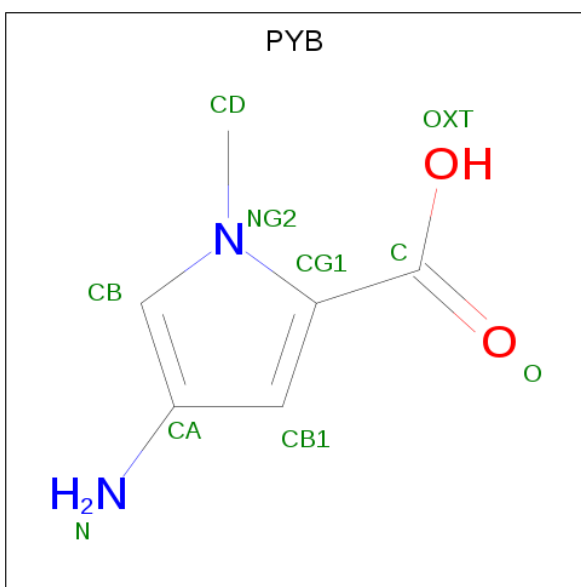
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	4	Total	Mn	0	0
			4	4		
6	I	6	Total	Mn	0	0
			6	6		
6	E	1	Total	Mn	0	0
			1	1		

- Molecule 7 is 4-AMINO-(1-METHYLIMIDAZOLE)-2-CARBOXYLIC ACID (three-letter code: IMT) (formula: C₅H₇N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	I	1	Total	C	N	O	0	0
			8	5	2	1		
7	I	1	Total	C	N	O	0	0
			8	5	2	1		
7	J	1	Total	C	N	O	0	0
			8	5	2	1		
7	J	1	Total	C	N	O	0	0
			8	5	2	1		
7	J	1	Total	C	N	O	0	0
			8	5	2	1		

- Molecule 8 is 4-AMINO-(1-METHYLPYRROLE)-2-CARBOXYLIC ACID (three-letter code: PYB) (formula: C₆H₈N₂O₂).



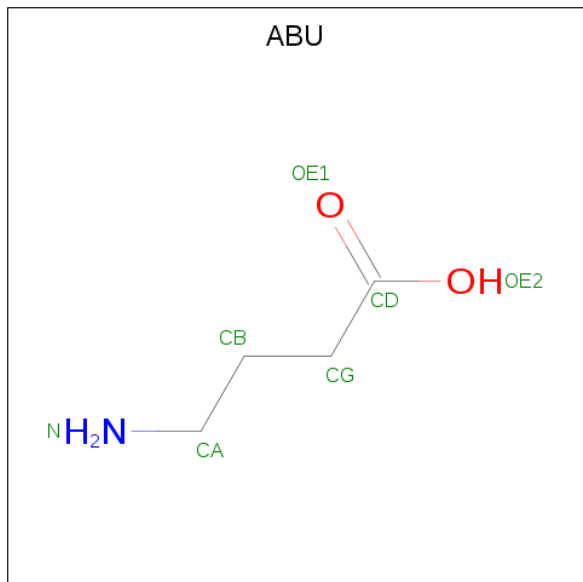
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		
8	I	1	Total	C	N	O	0	0
			9	6	2	1		

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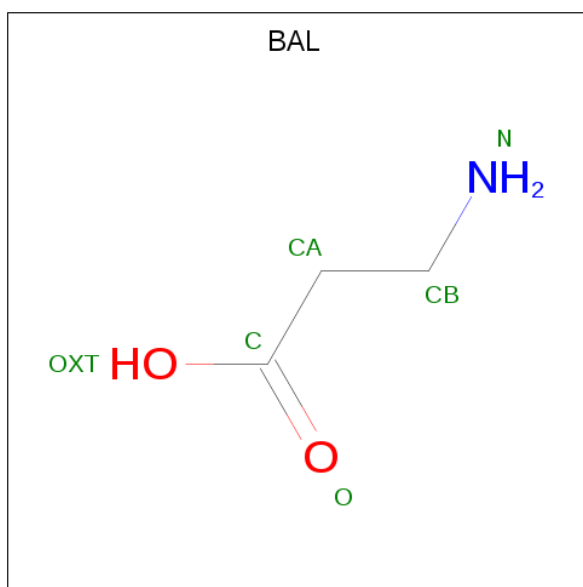
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		

- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



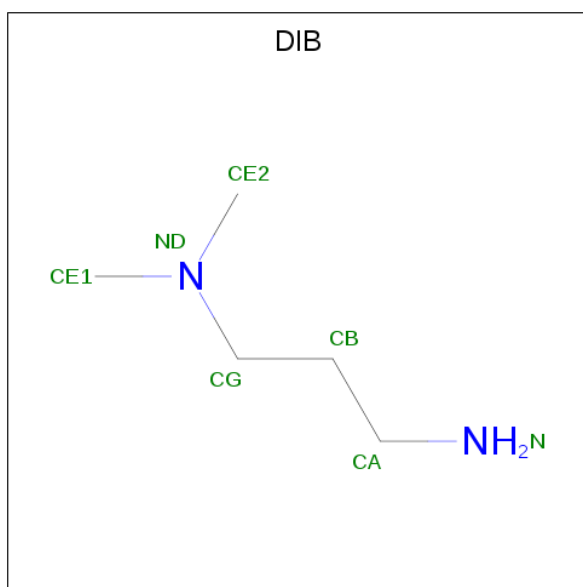
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	1	Total	C	N	O	0	0
			6	4	1	1		
9	I	1	Total	C	N	O	0	0
			6	4	1	1		
9	J	1	Total	C	N	O	0	0
			6	4	1	1		
9	J	1	Total	C	N	O	0	0
			6	4	1	1		
9	J	1	Total	C	N	O	0	0
			6	4	1	1		

- Molecule 10 is BETA-ALANINE (three-letter code: BAL) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	I	1	Total	C	N	O	0	0
			5	3	1	1		
10	I	1	Total	C	N	O	0	0
			5	3	1	1		
10	J	1	Total	C	N	O	0	0
			5	3	1	1		
10	J	1	Total	C	N	O	0	0
			5	3	1	1		
10	J	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 11 is 3-AMINO-(DIMETHYLPROPYLAMINE) (three-letter code: DIB) (formula: C₅H₁₄N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	I	1	Total	C	N	0	0
			7	5	2		
11	I	1	Total	C	N	0	0
			7	5	2		
11	J	1	Total	C	N	0	0
			7	5	2		
11	J	1	Total	C	N	0	0
			7	5	2		
11	J	1	Total	C	N	0	0
			7	5	2		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	88	Total	O	0	0
			88	88		
12	J	67	Total	O	0	0
			67	67		
12	A	68	Total	O	0	0
			68	68		
12	B	46	Total	O	0	0
			46	46		
12	C	79	Total	O	0	0
			79	79		
12	D	44	Total	O	0	0
			44	44		
12	E	84	Total	O	0	0
			84	84		

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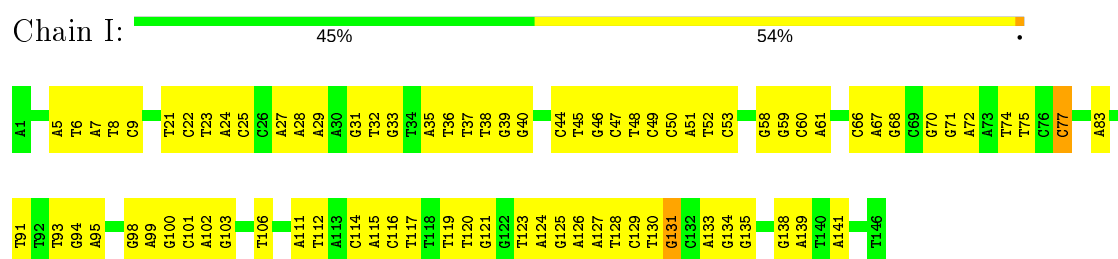
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	F	75	Total 75	O 75	0	0
12	G	66	Total 66	O 66	0	0
12	H	40	Total 40	O 40	0	0

3 Residue-property plots

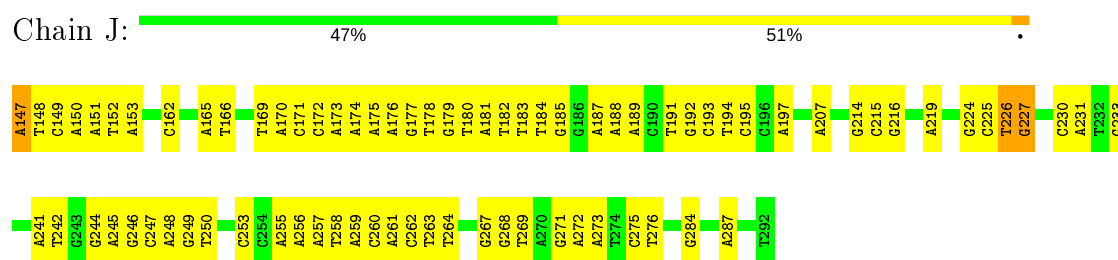
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

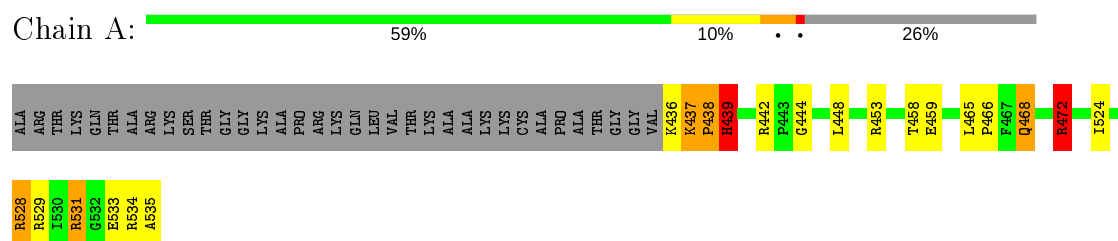
• Molecule 1: Palindromic 146 Base Pair DNA Fragment



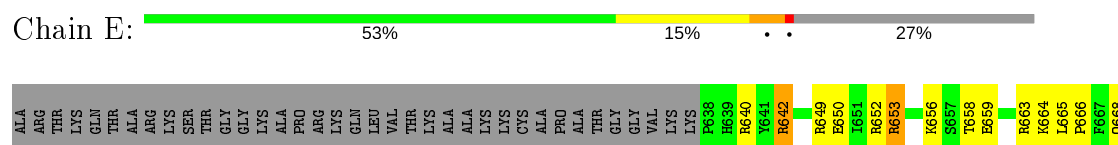
• Molecule 1: Palindromic 146 Base Pair DNA Fragment



• Molecule 2: Histone H3.2



• Molecule 2: Histone H3.2





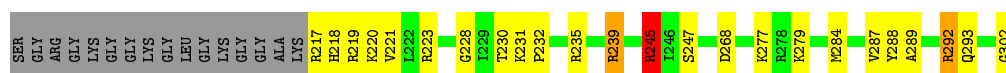
- Molecule 3: Histone H4

Chain B: 64% 13% 23%



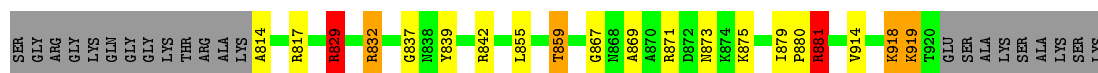
- Molecule 3: Histone H4

Chain F: 61% 21% 16%



- Molecule 4: Histone H2A.1

Chain C: 67% 11% 17%



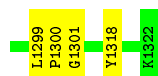
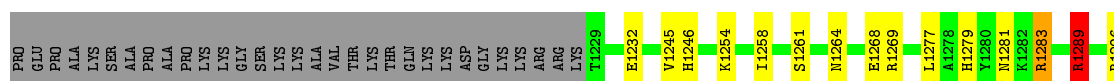
- Molecule 4: Histone H2A.1

Chain G: 63% 15% 19%



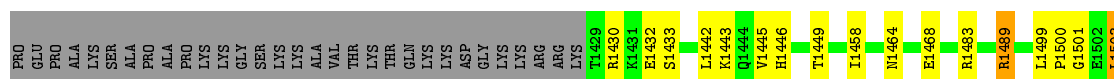
- Molecule 5: Histone H2B.1

Chain D: 60% 14% 25%



- Molecule 5: Histone H2B.1

Chain H: 62% 12% 25%



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K1522

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.05Å 109.66Å 183.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.30	Depositor
% Data completeness (in resolution range)	97.1 (80.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13158	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, DIB, IMT, BAL, PYB, ABU

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	I	0.50	0/3354	0.77	0/5175
1	J	0.52	0/3354	0.80	1/5175 (0.0%)
2	A	0.70	0/838	0.88	3/1122 (0.3%)
2	E	0.86	0/820	1.01	4/1099 (0.4%)
3	B	0.74	0/634	0.93	1/848 (0.1%)
3	F	0.86	0/702	0.97	1/937 (0.1%)
4	C	0.76	0/835	0.85	1/1127 (0.1%)
4	G	0.65	0/823	0.76	1/1110 (0.1%)
5	D	0.77	0/747	0.84	0/1004
5	H	0.68	0/747	0.79	0/1004
All	All	0.64	0/12854	0.83	12/18601 (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
1	I	0	4
1	J	0	3
2	A	0	2
2	E	0	2
3	B	0	2
3	F	0	2
4	C	0	1
4	G	0	2
5	D	0	1
All	All	0	19

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	245	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	E	728	ARG	NE-CZ-NH2	-7.55	116.53	120.30
2	E	672	ARG	NE-CZ-NH2	-7.51	116.55	120.30
3	B	36	ARG	NE-CZ-NH1	-6.62	116.99	120.30
4	G	1081	ARG	NE-CZ-NH2	-6.49	117.06	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	131	DG	Sidechain
1	I	135	DG	Sidechain
1	I	67	DA	Sidechain
1	I	77	DC	Sidechain
1	J	147	DA	Sidechain

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	I	2990	0	1651	132	0
1	J	2990	0	1651	132	0
2	A	826	0	871	16	0
2	E	808	0	846	23	0
3	B	627	0	663	9	0
3	F	694	0	742	18	0
4	C	825	0	884	23	0
4	G	813	0	872	32	0
5	D	736	0	760	15	0
5	H	736	0	760	15	0
6	E	1	0	0	0	0
6	I	6	0	0	0	0
6	J	4	0	0	0	0
7	I	16	0	8	8	0
7	J	24	0	12	10	0
8	I	126	0	84	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	189	0	126	75	0
9	I	12	0	12	4	0
9	J	18	0	18	14	0
10	I	10	0	8	3	0
10	J	15	0	12	2	0
11	I	14	0	25	5	0
11	J	21	0	37	8	0
12	A	68	0	0	1	0
12	B	46	0	0	3	0
12	C	79	0	0	3	0
12	D	44	0	0	4	0
12	E	84	0	0	5	0
12	F	75	0	0	2	0
12	G	66	0	0	1	0
12	H	40	0	0	0	0
12	I	88	0	0	6	0
12	J	67	0	0	5	0
All	All	13158	0	10042	450	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 20.

The worst 5 of 450 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)
1:J:259:DA:C4'	9:J:1905:ABU:HG1	1.75	1.17
11:J:1911:DIB:HE22	4:C:814:ALA:HB3	1.36	1.08
1:J:249:DG:N2	8:J:1929:PYB:HB1	1.68	1.08
1:J:174:DA:H2''	1:J:175:DA:H5''	1.38	1.05
1:J:259:DA:H4'	9:J:1905:ABU:HG1	1.39	1.03

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	
2	A	98/135 (73%)	95 (97%)	1 (1%)	2 (2%)	7	6
2	E	96/135 (71%)	96 (100%)	0	0	100	100
3	B	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
3	F	84/102 (82%)	82 (98%)	1 (1%)	1 (1%)	13	14
4	C	105/129 (81%)	103 (98%)	1 (1%)	1 (1%)	15	17
4	G	103/129 (80%)	100 (97%)	3 (3%)	0	100	100
5	D	92/125 (74%)	90 (98%)	1 (1%)	1 (1%)	14	15
5	H	92/125 (74%)	90 (98%)	1 (1%)	1 (1%)	14	15
All	All	747/982 (76%)	732 (98%)	9 (1%)	6 (1%)	19	23

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	438	PRO
2	A	439	HIS
5	H	1501	GLY
4	C	919	LYS
5	D	1301	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	87/111 (78%)	79 (91%)	8 (9%)	9	11
2	E	85/111 (77%)	78 (92%)	7 (8%)	11	14
3	B	64/78 (82%)	61 (95%)	3 (5%)	26	37
3	F	71/78 (91%)	65 (92%)	6 (8%)	10	13
4	C	85/100 (85%)	80 (94%)	5 (6%)	19	27
4	G	84/100 (84%)	80 (95%)	4 (5%)	25	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	80/105 (76%)	77 (96%)	3 (4%)	33	47
5	H	80/105 (76%)	76 (95%)	4 (5%)	24	34
All	All	636/788 (81%)	596 (94%)	40 (6%)	18	24

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	1289	ARG
2	E	659	GLU
5	H	1433	SER
2	E	653	ARG
2	E	683	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	838	ASN
5	D	1264	ASN
5	D	1292	GLN
4	G	1031	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 11 are monoatomic - leaving 55 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PYB	I	2024	9,8	7,9,10	1.65	2 (28%)	3,12,14	3.20	2 (66%)
8	PYB	J	2002	8,7	7,9,10	1.54	1 (14%)	3,12,14	4.09	2 (66%)
8	PYB	I	2028	8	7,9,10	1.66	2 (28%)	3,12,14	3.56	2 (66%)
10	BAL	J	1910	11,8	4,4,5	0.52	0	3,3,5	1.37	0
8	PYB	J	1923	8	7,9,10	1.72	3 (42%)	3,12,14	3.78	2 (66%)
11	DIB	J	2011	10	6,6,6	0.70	0	6,6,6	0.56	0
8	PYB	I	1962	8,7	7,9,10	1.83	3 (42%)	3,12,14	4.18	2 (66%)
8	PYB	J	1904	9,8	7,9,10	1.96	3 (42%)	3,12,14	2.99	2 (66%)
8	PYB	I	1968	8	7,9,10	1.83	2 (28%)	3,12,14	4.12	2 (66%)
8	PYB	I	1963	8	7,9,10	1.71	2 (28%)	3,12,14	3.96	2 (66%)
8	PYB	J	2003	8	7,9,10	1.71	2 (28%)	3,12,14	3.72	2 (66%)
8	PYB	J	1908	8	7,9,10	1.71	2 (28%)	3,12,14	3.61	2 (66%)
9	ABU	I	2025	8	5,5,6	1.61	1 (20%)	4,4,6	0.43	0
7	IMT	J	2001	8	7,8,10	1.17	1 (14%)	5,10,14	2.62	3 (60%)
7	IMT	I	2021	8	7,8,10	1.07	1 (14%)	5,10,14	2.55	3 (60%)
8	PYB	I	2027	8	7,9,10	1.79	3 (42%)	3,12,14	3.96	2 (66%)
9	ABU	J	2005	8	5,5,6	1.62	1 (20%)	4,4,6	0.43	0
9	ABU	I	1965	8	5,5,6	1.60	1 (20%)	4,4,6	0.40	0
8	PYB	J	1924	9,8	7,9,10	1.67	2 (28%)	3,12,14	3.47	2 (66%)
8	PYB	I	1966	9,8	7,9,10	1.92	3 (42%)	3,12,14	3.67	2 (66%)
11	DIB	J	1931	10	6,6,6	0.74	0	6,6,6	0.41	0
8	PYB	J	2009	8,10	7,9,10	1.86	3 (42%)	3,12,14	3.43	2 (66%)
8	PYB	J	1928	8	7,9,10	1.53	1 (14%)	3,12,14	4.38	2 (66%)
8	PYB	J	1927	8	7,9,10	1.47	2 (28%)	3,12,14	4.19	2 (66%)
8	PYB	J	2004	9,8	7,9,10	1.69	2 (28%)	3,12,14	3.16	2 (66%)
8	PYB	I	2026	9,8	7,9,10	1.69	2 (28%)	3,12,14	3.72	2 (66%)
10	BAL	J	1930	11,8	4,4,5	0.52	0	3,3,5	1.33	0
8	PYB	J	1903	8	7,9,10	1.93	3 (42%)	3,12,14	3.77	2 (66%)
8	PYB	J	1922	8,7	7,9,10	1.68	2 (28%)	3,12,14	4.02	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PYB	J	1902	8,7	7,9,10	1.77	3 (42%)	3,12,14	3.94	2 (66%)
10	BAL	J	2010	11,8	4,4,5	0.67	0	3,3,5	1.79	1 (33%)
9	ABU	J	1905	8	5,5,6	1.65	1 (20%)	4,4,6	0.42	0
7	IMT	I	1961	8	7,8,10	1.17	1 (14%)	5,10,14	2.52	3 (60%)
8	PYB	J	1909	8,10	7,9,10	1.91	3 (42%)	3,12,14	3.17	2 (66%)
11	DIB	J	1911	10	6,6,6	0.65	0	6,6,6	0.36	0
8	PYB	I	2029	8,10	7,9,10	1.66	2 (28%)	3,12,14	3.13	2 (66%)
8	PYB	I	1967	8	7,9,10	1.63	2 (28%)	3,12,14	3.84	2 (66%)
10	BAL	I	2030	11,8	4,4,5	0.56	0	3,3,5	1.47	1 (33%)
11	DIB	I	1971	10	6,6,6	0.73	0	6,6,6	0.46	0
8	PYB	J	1906	9,8	7,9,10	1.82	2 (28%)	3,12,14	4.12	2 (66%)
11	DIB	I	2031	10	6,6,6	0.71	0	6,6,6	0.45	0
7	IMT	J	1901	8	7,8,10	1.13	1 (14%)	5,10,14	2.55	3 (60%)
8	PYB	J	1926	9,8	7,9,10	1.72	2 (28%)	3,12,14	3.59	2 (66%)
8	PYB	J	1929	8,10	7,9,10	1.65	2 (28%)	3,12,14	3.48	2 (66%)
9	ABU	J	1925	8	5,5,6	1.61	1 (20%)	4,4,6	0.47	0
8	PYB	J	2008	8	7,9,10	1.65	2 (28%)	3,12,14	3.99	2 (66%)
10	BAL	I	1970	11,8	4,4,5	0.51	0	3,3,5	1.48	1 (33%)
8	PYB	J	1907	8	7,9,10	1.91	3 (42%)	3,12,14	3.81	2 (66%)
7	IMT	J	1921	8	7,8,10	1.36	1 (14%)	5,10,14	2.60	3 (60%)
8	PYB	I	2022	8,7	7,9,10	1.58	2 (28%)	3,12,14	4.21	2 (66%)
8	PYB	I	2023	8	7,9,10	1.70	3 (42%)	3,12,14	3.54	2 (66%)
8	PYB	I	1969	8,10	7,9,10	1.91	3 (42%)	3,12,14	3.01	2 (66%)
8	PYB	I	1964	9,8	7,9,10	1.93	3 (42%)	3,12,14	3.19	2 (66%)
8	PYB	J	2007	8	7,9,10	1.74	3 (42%)	3,12,14	3.64	2 (66%)
8	PYB	J	2006	9,8	7,9,10	1.70	2 (28%)	3,12,14	3.61	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PYB	I	2024	9,8	-	0/0/2/4	0/1/1/1
8	PYB	J	2002	8,7	-	0/0/2/4	0/1/1/1
8	PYB	I	2028	8	-	0/0/2/4	0/1/1/1
10	BAL	J	1910	11,8	-	0/1/2/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PYB	J	1923	8	-	0/0/2/4	0/1/1/1
11	DIB	J	2011	10	-	4/4/4/4	-
8	PYB	I	1962	8,7	-	0/0/2/4	0/1/1/1
8	PYB	J	1904	9,8	-	0/0/2/4	0/1/1/1
8	PYB	I	1968	8	-	0/0/2/4	0/1/1/1
8	PYB	I	1963	8	-	0/0/2/4	0/1/1/1
8	PYB	J	2003	8	-	0/0/2/4	0/1/1/1
8	PYB	J	1908	8	-	0/0/2/4	0/1/1/1
9	ABU	I	2025	8	-	3/3/3/4	-
7	IMT	J	2001	8	-	0/0/2/4	0/1/1/1
7	IMT	I	2021	8	-	0/0/2/4	0/1/1/1
8	PYB	I	2027	8	-	0/0/2/4	0/1/1/1
9	ABU	J	2005	8	-	3/3/3/4	-
9	ABU	I	1965	8	-	3/3/3/4	-
8	PYB	J	1924	9,8	-	0/0/2/4	0/1/1/1
8	PYB	I	1966	9,8	-	0/0/2/4	0/1/1/1
11	DIB	J	1931	10	-	1/4/4/4	-
8	PYB	J	2009	8,10	-	0/0/2/4	0/1/1/1
8	PYB	J	1928	8	-	0/0/2/4	0/1/1/1
8	PYB	J	1927	8	-	0/0/2/4	0/1/1/1
8	PYB	J	2004	9,8	-	0/0/2/4	0/1/1/1
8	PYB	I	2026	9,8	-	0/0/2/4	0/1/1/1
10	BAL	J	1930	11,8	-	0/1/2/3	-
8	PYB	J	1903	8	-	0/0/2/4	0/1/1/1
8	PYB	J	1922	8,7	-	0/0/2/4	0/1/1/1
8	PYB	J	1902	8,7	-	0/0/2/4	0/1/1/1
10	BAL	J	2010	11,8	-	0/1/2/3	-
9	ABU	J	1905	8	-	2/3/3/4	-
7	IMT	I	1961	8	-	0/0/2/4	0/1/1/1
8	PYB	J	1909	8,10	-	0/0/2/4	0/1/1/1
11	DIB	J	1911	10	-	3/4/4/4	-
8	PYB	I	2029	8,10	-	0/0/2/4	0/1/1/1
8	PYB	I	1967	8	-	0/0/2/4	0/1/1/1
10	BAL	I	2030	11,8	-	0/1/2/3	-
11	DIB	I	1971	10	-	0/4/4/4	-
8	PYB	J	1906	9,8	-	0/0/2/4	0/1/1/1
11	DIB	I	2031	10	-	1/4/4/4	-
7	IMT	J	1901	8	-	0/0/2/4	0/1/1/1
8	PYB	J	1926	9,8	-	0/0/2/4	0/1/1/1
8	PYB	J	1929	8,10	-	0/0/2/4	0/1/1/1
9	ABU	J	1925	8	-	3/3/3/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PYB	J	2008	8	-	0/0/2/4	0/1/1/1
10	BAL	I	1970	11,8	-	0/1/2/3	-
8	PYB	J	1907	8	-	0/0/2/4	0/1/1/1
7	IMT	J	1921	8	-	0/0/2/4	0/1/1/1
8	PYB	I	2022	8,7	-	0/0/2/4	0/1/1/1
8	PYB	I	2023	8	-	0/0/2/4	0/1/1/1
8	PYB	I	1969	8,10	-	0/0/2/4	0/1/1/1
8	PYB	I	1964	9,8	-	0/0/2/4	0/1/1/1
8	PYB	J	2007	8	-	0/0/2/4	0/1/1/1
8	PYB	J	2006	9,8	-	0/0/2/4	0/1/1/1

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	1905	ABU	OE2-CD	-3.68	1.23	1.42
9	I	2025	ABU	OE2-CD	-3.57	1.23	1.42
9	J	1925	ABU	OE2-CD	-3.56	1.23	1.42
9	J	2005	ABU	OE2-CD	-3.55	1.23	1.42
8	J	1909	PYB	CG1-NG2	3.49	1.43	1.36

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1962	PYB	O-C-CG1	-6.41	115.09	124.17
8	I	2022	PYB	O-C-CG1	-6.25	115.31	124.17
8	J	1902	PYB	O-C-CG1	-6.22	115.36	124.17
8	I	1963	PYB	O-C-CG1	-6.19	115.40	124.17
8	I	1968	PYB	O-C-CG1	-6.12	115.50	124.17

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	J	2011	DIB	CB-CG-ND-CE1
11	J	2011	DIB	CB-CG-ND-CE2
11	J	1911	DIB	CB-CG-ND-CE1
11	J	2011	DIB	CA-CB-CG-ND
11	J	1931	DIB	CA-CB-CG-ND

There are no ring outliers.

53 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	2024	PYB	4	0
8	J	2002	PYB	4	0
8	I	2028	PYB	6	0
8	J	1923	PYB	4	0
11	J	2011	DIB	2	0
8	I	1962	PYB	5	0
8	J	1904	PYB	4	0
8	I	1968	PYB	5	0
8	I	1963	PYB	5	0
8	J	2003	PYB	7	0
8	J	1908	PYB	7	0
9	I	2025	ABU	3	0
7	J	2001	IMT	3	0
7	I	2021	IMT	3	0
8	I	2027	PYB	3	0
9	J	2005	ABU	3	0
9	I	1965	ABU	1	0
8	J	1924	PYB	4	0
8	I	1966	PYB	3	0
11	J	1931	DIB	3	0
8	J	2009	PYB	5	0
8	J	1928	PYB	8	0
8	J	1927	PYB	5	0
8	J	2004	PYB	3	0
8	I	2026	PYB	3	0
10	J	1930	BAL	1	0
8	J	1903	PYB	6	0
8	J	1922	PYB	4	0
8	J	1902	PYB	5	0
10	J	2010	BAL	1	0
9	J	1905	ABU	11	0
7	I	1961	IMT	5	0
8	J	1909	PYB	2	0
11	J	1911	DIB	3	0
8	I	2029	PYB	10	0
8	I	1967	PYB	5	0
10	I	2030	BAL	2	0
11	I	1971	DIB	2	0
8	J	1906	PYB	6	0
11	I	2031	DIB	3	0
7	J	1901	IMT	5	0
8	J	1926	PYB	2	0
8	J	1929	PYB	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	2008	PYB	6	0
10	I	1970	BAL	1	0
8	J	1907	PYB	5	0
7	J	1921	IMT	2	0
8	I	2022	PYB	5	0
8	I	2023	PYB	5	0
8	I	1969	PYB	5	0
8	I	1964	PYB	4	0
8	J	2007	PYB	4	0
8	J	2006	PYB	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.