



wwPDB EM Validation Summary Report ⓘ

Mar 3, 2025 – 06:04 pm GMT

PDB ID : 9GMK
EMDB ID : EMD-51449
Title : SIRT7:H3K18DTU nucleosome complex
Authors : Moreno-Yruela, C.; Ekundayo, B.; Foteva, P.; Calvino-Sanles, E.; Ni, D.;
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Deposited on : 2024-08-29
Resolution : 3.50 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

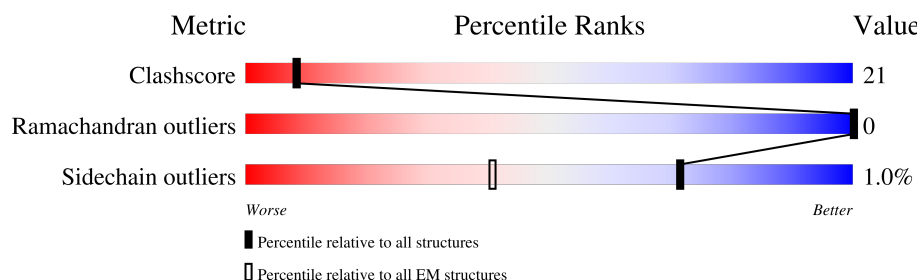
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	136	35% 35% . 30%
1	E	136	42% 29% 29%
2	B	103	38% 43% 19%
2	F	103	42% 34% 24%
3	C	129	44% 36% 19%
3	G	129	52% 29% . 19%
4	D	126	38% 33% . 27%
4	H	126	36% 38% 26%
5	K	401	41% 41% . 17%

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Mol	Chain	Length	Quality of chain
6	L	148	 45% 55%
7	M	148	 28% 72%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14643 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	95	Total	C	N	O	S	0	0
			784	494	151	136	3		
1	E	97	Total	C	N	O	S	0	0
			800	503	155	139	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	CYS	ALA	conflict	UNP Q71DI3
A	110	ALA	CYS	conflict	UNP Q71DI3
E	47	CYS	ALA	conflict	UNP Q71DI3
E	110	ALA	CYS	conflict	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	F	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 3 is a protein called Histone H2A type 2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	104	Total	C	N	O	S	0	0
			801	506	155	139	1		
3	G	105	Total	C	N	O	S	0	0
			806	509	156	140	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	92	Total	C	N	O	S	0	0
			717	453	127	135	2		
4	H	93	Total	C	N	O	S	0	0
			724	456	130	136	2		

- Molecule 5 is a protein called NAD-dependent protein deacetylase sirtuin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	334	Total	C	N	O	S	0	0
			2662	1642	516	489	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP Q9NRC8

- Molecule 6 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	148	Total	C	N	O	P	0	0
			3014	1436	535	895	148		

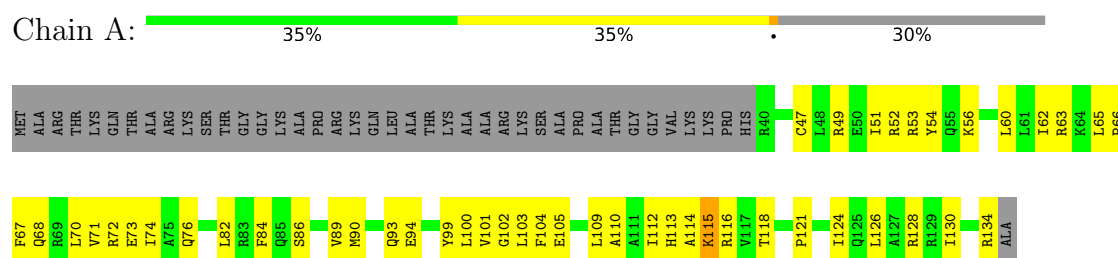
- Molecule 7 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	148	Total	C	N	O	P	0	0
			3054	1447	578	881	148		

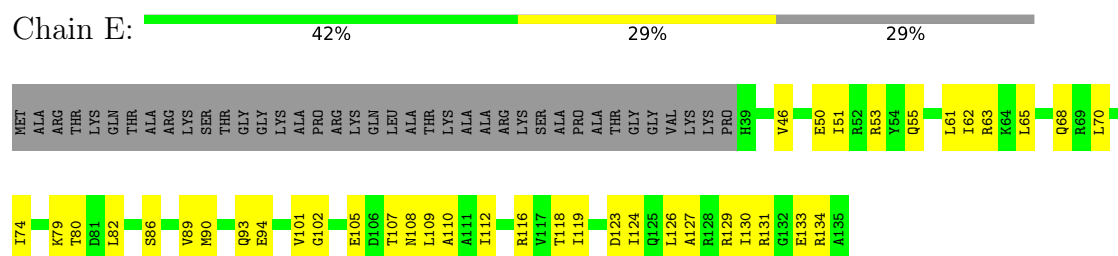
3 Residue-property plots [i](#)

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. 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.

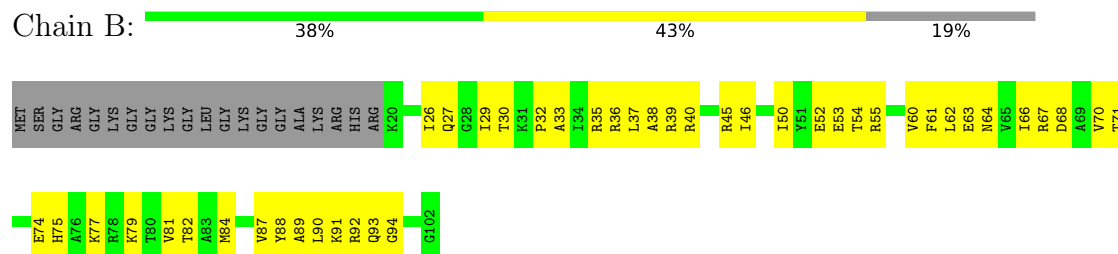
• Molecule 1: Histone H3.2



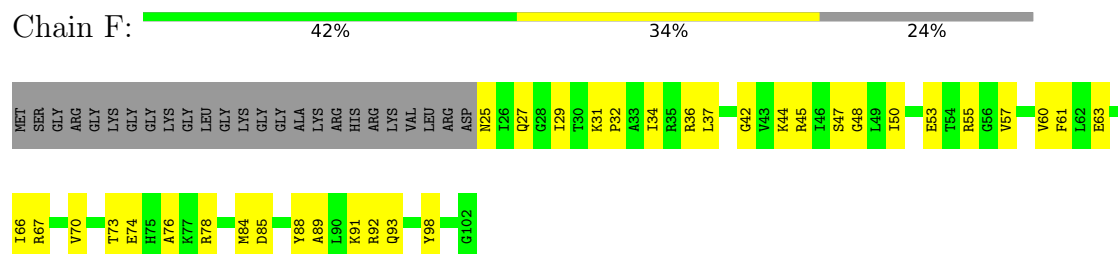
• Molecule 1: Histone H3.2



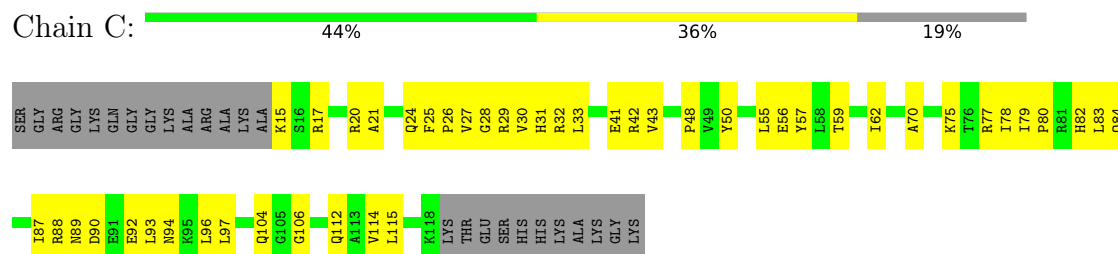
• Molecule 2: Histone H4



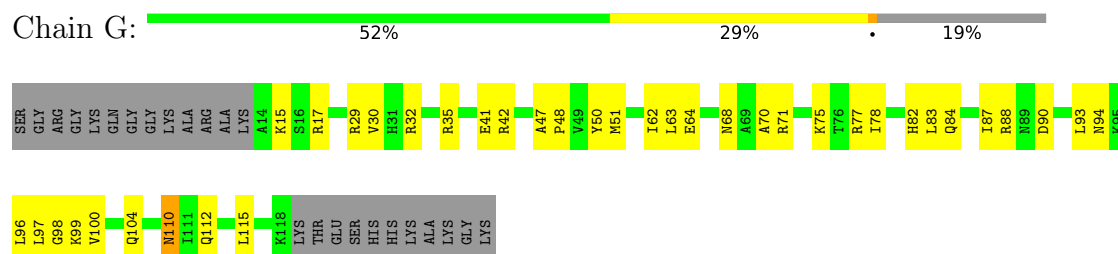
• Molecule 2: Histone H4



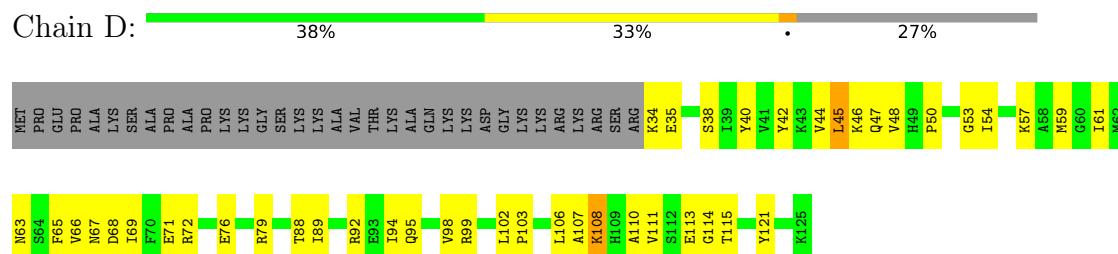
- Molecule 3: Histone H2A type 2-A



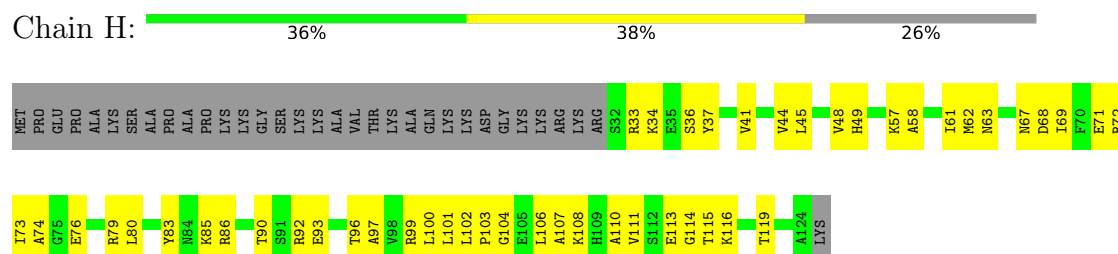
- Molecule 3: Histone H2A type 2-A



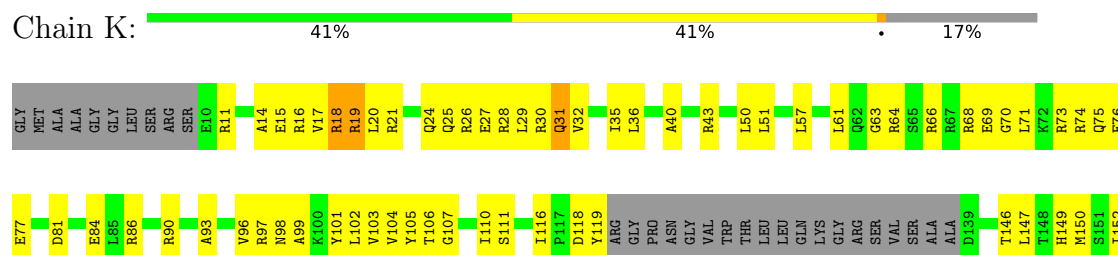
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J

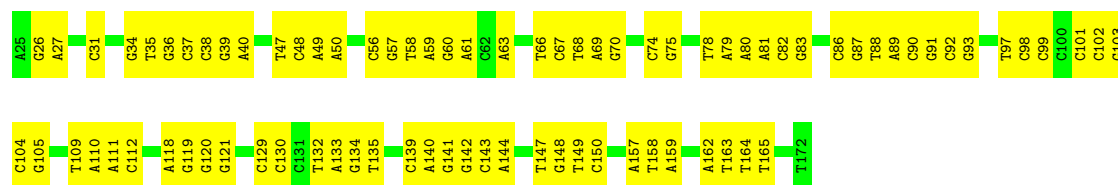


- Molecule 5: NAD-dependent protein deacetylase sirtuin-7

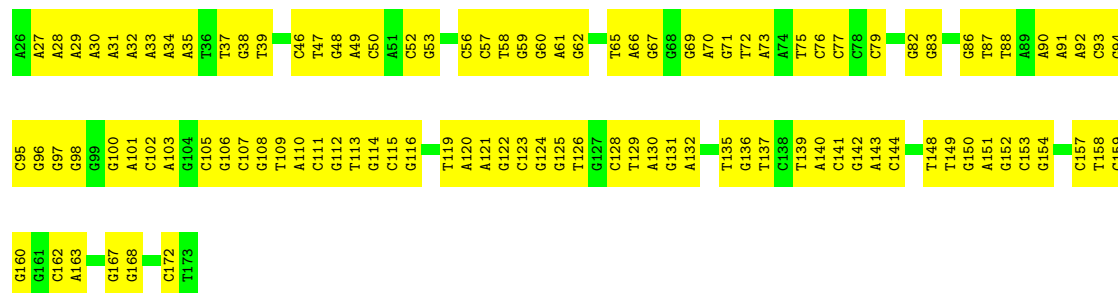




• Molecule 6: DNA (148-MER)



• Molecule 7: DNA (148-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22579	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/794	0.66	0/1064
1	E	0.29	0/811	0.63	0/1086
2	B	0.29	0/669	0.64	0/894
2	F	0.30	0/626	0.65	0/837
3	C	0.30	0/811	0.58	0/1093
3	G	0.26	0/816	0.58	0/1100
4	D	0.31	0/728	0.65	2/978 (0.2%)
4	H	0.32	0/735	0.62	0/989
5	K	0.26	0/2706	0.59	0/3648
6	L	0.50	0/3374	0.93	0/5201
7	M	0.48	0/3432	0.87	0/5299
All	All	0.39	0/15502	0.76	2/22189 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	45	LEU	CA-CB-CG	5.38	127.66	115.30
4	D	45	LEU	CB-CG-CD2	-5.05	102.42	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	784	0	824	45	0
1	E	800	0	836	39	0
2	B	662	0	709	43	0
2	F	619	0	659	35	0
3	C	801	0	857	50	0
3	G	806	0	862	33	0
4	D	717	0	737	46	0
4	H	724	0	742	44	0
5	K	2662	0	2694	136	0
6	L	3014	0	1668	72	0
7	M	3054	0	1661	102	0
All	All	14643	0	12249	564	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 21.

The worst 5 of 564 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:A:130:ILE:HD12	1:E:130:ILE:HD13	1.57	0.86
5:K:274:LEU:HB3	5:K:281:TRP:HE1	1.42	0.82
6:L:26:DG:N2	7:M:172:DC:O2	2.13	0.81
6:L:26:DG:N1	7:M:172:DC:N3	2.29	0.80
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.16	0.79

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 PDB entries followed by that with respect to all EM entries.

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	93/136 (68%)	90 (97%)	3 (3%)	0	100	100
1	E	95/136 (70%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	F	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
3	C	102/129 (79%)	100 (98%)	2 (2%)	0	100	100
3	G	103/129 (80%)	100 (97%)	3 (3%)	0	100	100
4	D	90/126 (71%)	88 (98%)	2 (2%)	0	100	100
4	H	91/126 (72%)	87 (96%)	4 (4%)	0	100	100
5	K	330/401 (82%)	327 (99%)	3 (1%)	0	100	100
All	All	1061/1389 (76%)	1040 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	83/111 (75%)	82 (99%)	1 (1%)	67	82
1	E	84/111 (76%)	84 (100%)	0	100	100
2	B	68/79 (86%)	68 (100%)	0	100	100
2	F	63/79 (80%)	63 (100%)	0	100	100
3	C	82/98 (84%)	82 (100%)	0	100	100
3	G	82/98 (84%)	81 (99%)	1 (1%)	67	82
4	D	77/105 (73%)	76 (99%)	1 (1%)	65	81
4	H	78/105 (74%)	77 (99%)	1 (1%)	65	81
5	K	286/335 (85%)	281 (98%)	5 (2%)	56	75
All	All	903/1121 (81%)	894 (99%)	9 (1%)	71	84

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	97	ARG

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Mol	Chain	Res	Type
5	K	218	ARG
4	H	63	ASN
5	K	18	ARG
5	K	19	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	68	ASN
5	K	173	HIS
5	K	189	ASN
1	E	93	GLN
3	C	82	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.