



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:49 AM BST

PDB ID : 5Z9R
Title : NMNAT as a specific chaperone antagonizing pathological condensation of phosphorylated tau
Authors : Dou, S.; Ma, X.; Li, D.; Liu, C.
Deposited on : 2018-02-05
Resolution : 2.00 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 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	:	2.13
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)	:	2.13

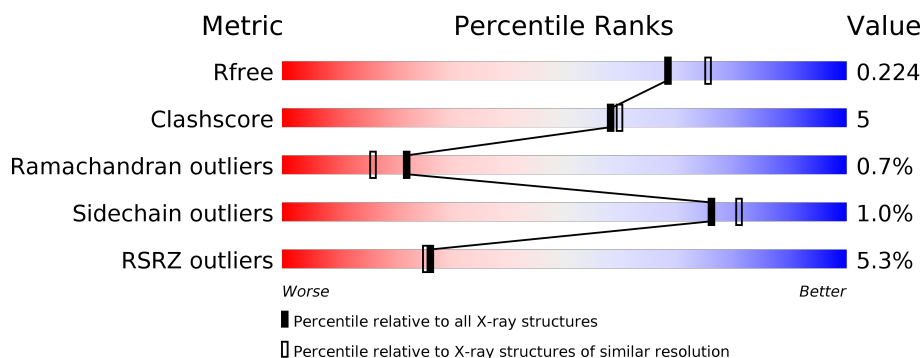
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	281	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>9%</div> <div>23%</div> </div> </div>
1	B	281	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>8%</div> <div>22%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3733 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 Nicotinamide/nicotinic acid mononucleotide adenylyltransferase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1755	1115	320	314	6			
1	B	218	Total	C	N	O	S	0	0	0
			1763	1120	321	315	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP Q99JR6
A	-34	GLY	-	expression tag	UNP Q99JR6
A	-33	SER	-	expression tag	UNP Q99JR6
A	-32	SER	-	expression tag	UNP Q99JR6
A	-31	HIS	-	expression tag	UNP Q99JR6
A	-30	HIS	-	expression tag	UNP Q99JR6
A	-29	HIS	-	expression tag	UNP Q99JR6
A	-28	HIS	-	expression tag	UNP Q99JR6
A	-27	HIS	-	expression tag	UNP Q99JR6
A	-26	HIS	-	expression tag	UNP Q99JR6
A	-25	SER	-	expression tag	UNP Q99JR6
A	-24	SER	-	expression tag	UNP Q99JR6
A	-23	GLY	-	expression tag	UNP Q99JR6
A	-22	LEU	-	expression tag	UNP Q99JR6
A	-21	VAL	-	expression tag	UNP Q99JR6
A	-20	PRO	-	expression tag	UNP Q99JR6
A	-19	ARG	-	expression tag	UNP Q99JR6
A	-18	GLY	-	expression tag	UNP Q99JR6
A	-17	SER	-	expression tag	UNP Q99JR6
A	-16	HIS	-	expression tag	UNP Q99JR6
A	-15	MET	-	expression tag	UNP Q99JR6
A	-14	ALA	-	expression tag	UNP Q99JR6
A	-13	SER	-	expression tag	UNP Q99JR6
A	-12	MET	-	expression tag	UNP Q99JR6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	THR	-	expression tag	UNP Q99JR6
A	-10	GLY	-	expression tag	UNP Q99JR6
A	-9	GLY	-	expression tag	UNP Q99JR6
A	-8	GLN	-	expression tag	UNP Q99JR6
A	-7	GLN	-	expression tag	UNP Q99JR6
A	-6	MET	-	expression tag	UNP Q99JR6
A	-5	GLY	-	expression tag	UNP Q99JR6
A	-4	ARG	-	expression tag	UNP Q99JR6
A	-3	GLY	-	expression tag	UNP Q99JR6
A	-2	SER	-	expression tag	UNP Q99JR6
A	-1	GLU	-	expression tag	UNP Q99JR6
A	0	PHE	-	expression tag	UNP Q99JR6
B	-35	MET	-	expression tag	UNP Q99JR6
B	-34	GLY	-	expression tag	UNP Q99JR6
B	-33	SER	-	expression tag	UNP Q99JR6
B	-32	SER	-	expression tag	UNP Q99JR6
B	-31	HIS	-	expression tag	UNP Q99JR6
B	-30	HIS	-	expression tag	UNP Q99JR6
B	-29	HIS	-	expression tag	UNP Q99JR6
B	-28	HIS	-	expression tag	UNP Q99JR6
B	-27	HIS	-	expression tag	UNP Q99JR6
B	-26	HIS	-	expression tag	UNP Q99JR6
B	-25	SER	-	expression tag	UNP Q99JR6
B	-24	SER	-	expression tag	UNP Q99JR6
B	-23	GLY	-	expression tag	UNP Q99JR6
B	-22	LEU	-	expression tag	UNP Q99JR6
B	-21	VAL	-	expression tag	UNP Q99JR6
B	-20	PRO	-	expression tag	UNP Q99JR6
B	-19	ARG	-	expression tag	UNP Q99JR6
B	-18	GLY	-	expression tag	UNP Q99JR6
B	-17	SER	-	expression tag	UNP Q99JR6
B	-16	HIS	-	expression tag	UNP Q99JR6
B	-15	MET	-	expression tag	UNP Q99JR6
B	-14	ALA	-	expression tag	UNP Q99JR6
B	-13	SER	-	expression tag	UNP Q99JR6
B	-12	MET	-	expression tag	UNP Q99JR6
B	-11	THR	-	expression tag	UNP Q99JR6
B	-10	GLY	-	expression tag	UNP Q99JR6
B	-9	GLY	-	expression tag	UNP Q99JR6
B	-8	GLN	-	expression tag	UNP Q99JR6
B	-7	GLN	-	expression tag	UNP Q99JR6
B	-6	MET	-	expression tag	UNP Q99JR6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q99JR6
B	-4	ARG	-	expression tag	UNP Q99JR6
B	-3	GLY	-	expression tag	UNP Q99JR6
B	-2	SER	-	expression tag	UNP Q99JR6
B	-1	GLU	-	expression tag	UNP Q99JR6
B	0	PHE	-	expression tag	UNP Q99JR6

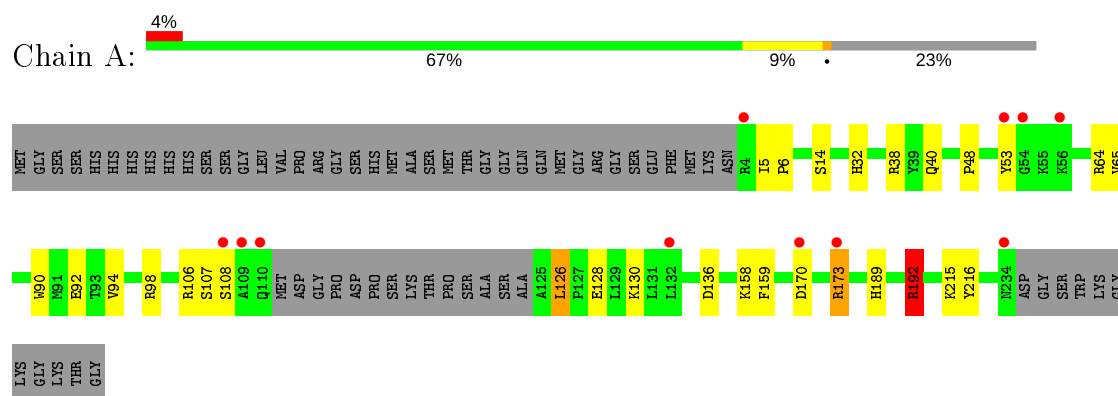
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	109	Total O 109 109	0	0
2	B	106	Total O 106 106	0	0

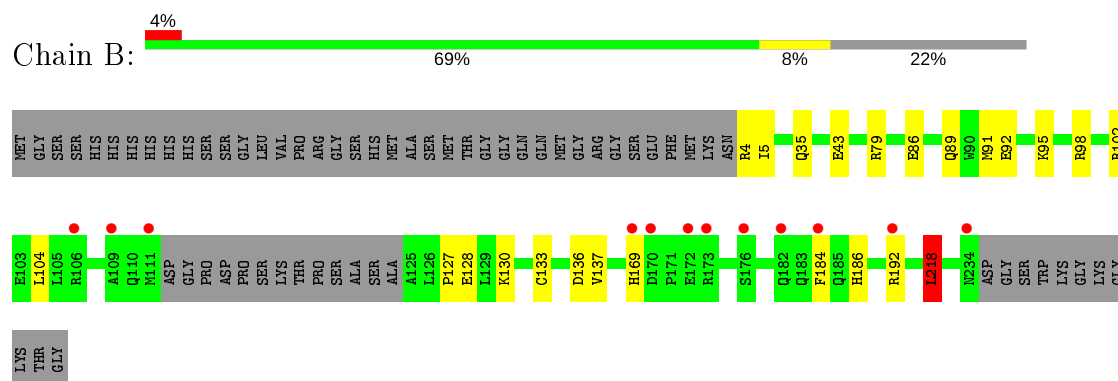
3 Residue-property plots [i](#)

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: Nicotinamide/nicotinic acid mononucleotide adenylyltransferase 3



- Molecule 1: Nicotinamide/nicotinic acid mononucleotide adenylyltransferase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.65Å 80.82Å 64.50Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	31.52 – 2.00 34.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (31.52-2.00) 98.2 (34.02-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.191 , 0.224 0.191 , 0.224	Depositor DCC
R_{free} test set	1796 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3733	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	4/1795 (0.2%)	0.58	1/2436 (0.0%)
1	B	0.36	0/1803	0.53	1/2446 (0.0%)
All	All	0.45	4/3598 (0.1%)	0.55	2/4882 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ARG	CZ-NH1	-9.39	1.20	1.33
1	A	192	ARG	NE-CZ	-8.26	1.22	1.33
1	A	192	ARG	CZ-NH2	-6.18	1.25	1.33
1	A	192	ARG	CD-NE	-5.27	1.37	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	LEU	CA-CB-CG	7.21	131.88	115.30
1	B	218	LEU	CA-CB-CG	5.46	127.87	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1755	0	1761	18	0
1	B	1763	0	1770	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	109	0	0	2	0
2	B	106	0	0	4	0
All	All	3733	0	3531	34	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 5.

All (34) 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:B:192:ARG:NH2	2:B:304:HOH:O	2.22	0.70
1:B:86:GLU:OE1	2:B:301:HOH:O	2.13	0.65
1:A:170:ASP:CG	1:A:173:ARG:HG2	2.18	0.64
1:A:48:PRO:HG2	1:A:65:VAL:HG12	1.79	0.63
1:B:104:LEU:HD21	1:B:127:PRO:HB2	1.81	0.61
1:A:128:GLU:OE1	1:A:130:LYS:NZ	2.36	0.58
1:B:43:GLU:OE2	2:B:302:HOH:O	2.16	0.58
1:A:192:ARG:NH2	2:A:301:HOH:O	2.21	0.56
1:A:136:ASP:N	1:A:136:ASP:OD1	2.41	0.54
1:A:106:ARG:C	1:A:108:SER:H	2.12	0.54
1:A:5:ILE:HD11	1:A:128:GLU:HG3	1.91	0.52
1:A:5:ILE:HG22	1:A:38:ARG:O	2.09	0.52
1:B:128:GLU:OE1	1:B:130:LYS:NZ	2.44	0.50
1:B:133:CYS:HB2	1:B:137:VAL:HG21	1.92	0.50
1:B:98:ARG:O	1:B:102:ARG:HG3	2.12	0.49
1:A:215:LYS:HD3	1:A:216:TYR:CZ	2.49	0.48
1:B:43:GLU:OE1	1:B:79:ARG:NE	2.29	0.48
1:A:90:TRP:CH2	1:A:92:GLU:HG3	2.49	0.47
1:B:92:GLU:OE2	2:B:303:HOH:O	2.20	0.47
1:A:130:LYS:HE2	1:A:189:HIS:NE2	2.29	0.47
1:A:94:VAL:O	1:A:98:ARG:HG3	2.16	0.46
1:B:89:GLN:HG3	1:B:91:MET:HE2	1.98	0.45
1:A:32:HIS:ND1	1:A:192:ARG:NH1	2.65	0.45
1:A:158:LYS:HG2	1:A:159:PHE:CE2	2.52	0.44
1:B:136:ASP:HB3	1:B:169:HIS:CE1	2.53	0.44
1:B:4:ARG:HD2	1:B:4:ARG:HA	1.62	0.43
1:B:218:LEU:N	1:B:218:LEU:HD12	2.35	0.42
1:A:14:SER:O	1:A:64:ARG:HD2	2.20	0.41
1:B:184:PHE:CD2	1:B:186:HIS:NE2	2.88	0.41
1:B:5:ILE:HG21	1:B:128:GLU:OE2	2.20	0.41
1:B:92:GLU:H	1:B:95:LYS:NZ	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PRO:HA	1:A:40:GLN:O	2.21	0.41
1:A:158:LYS:HG3	1:A:158:LYS:O	2.21	0.40
1:A:92:GLU:HG2	2:A:356:HOH:O	2.22	0.40

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	213/281 (76%)	206 (97%)	4 (2%)	3 (1%)	11	5
1	B	214/281 (76%)	209 (98%)	5 (2%)	0	100	100
All	All	427/562 (76%)	415 (97%)	9 (2%)	3 (1%)	22	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	TYR
1	A	126	LEU
1	A	107	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/242 (80%)	191 (99%)	2 (1%)	76	81
1	B	194/242 (80%)	192 (99%)	2 (1%)	76	81
All	All	387/484 (80%)	383 (99%)	4 (1%)	76	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	192	ARG
1	B	35	GLN
1	B	218	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	B	20	ASN
1	B	110	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	217/281 (77%)	0.45	11 (5%)	28 27	31, 42, 68, 93	0
1	B	218/281 (77%)	0.07	12 (5%)	25 24	31, 44, 70, 75	0
All	All	435/562 (77%)	0.26	23 (5%)	26 25	31, 43, 68, 93	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	10.7
1	A	110	GLN	7.8
1	A	173	ARG	6.5
1	A	234	ASN	4.4
1	A	53	TYR	4.1
1	B	184	PHE	3.8
1	B	111	MET	3.7
1	A	56	LYS	3.2
1	A	54	GLY	3.2
1	B	172	GLU	3.0
1	B	173	ARG	3.0
1	A	4	ARG	2.9
1	B	234	ASN	2.9
1	A	108	SER	2.7
1	B	176	SER	2.6
1	B	182	GLN	2.5
1	B	170	ASP	2.4
1	A	170	ASP	2.3
1	A	132	LEU	2.2
1	B	106	ARG	2.2
1	B	169	HIS	2.1
1	B	109	ALA	2.0
1	B	192	ARG	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.