



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:25 pm BST

PDB ID : 6D6K
Title : Structure of polyribonucleotide nucleotidyltransferase from *Acinetobacter baumannii*
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-04-21
Resolution : 2.50 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	:	2.11
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)	:	2.11

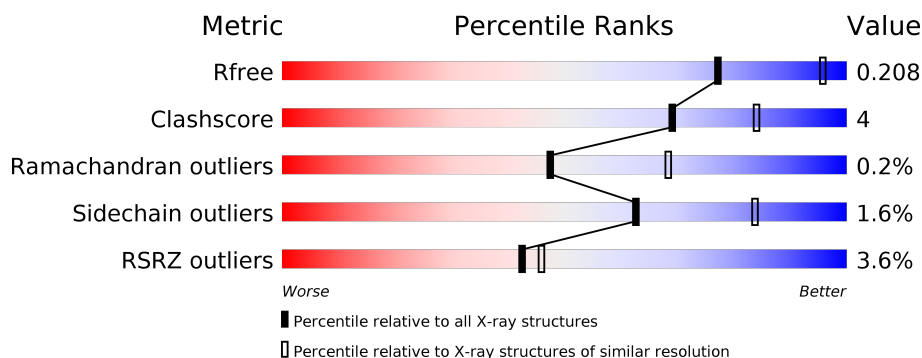
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	705	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>8%</div> <div>23%</div> </div> </div>
1	B	705	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>6%</div> <div>22%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8614 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 Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	2	0
			4004	2510	698	776	20			
1	B	552	Total	C	N	O	S	0	2	0
			4105	2577	715	793	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP V5VH92
A	-6	ALA	-	expression tag	UNP V5VH92
A	-5	HIS	-	expression tag	UNP V5VH92
A	-4	HIS	-	expression tag	UNP V5VH92
A	-3	HIS	-	expression tag	UNP V5VH92
A	-2	HIS	-	expression tag	UNP V5VH92
A	-1	HIS	-	expression tag	UNP V5VH92
A	0	HIS	-	expression tag	UNP V5VH92
B	-7	MET	-	initiating methionine	UNP V5VH92
B	-6	ALA	-	expression tag	UNP V5VH92
B	-5	HIS	-	expression tag	UNP V5VH92
B	-4	HIS	-	expression tag	UNP V5VH92
B	-3	HIS	-	expression tag	UNP V5VH92
B	-2	HIS	-	expression tag	UNP V5VH92
B	-1	HIS	-	expression tag	UNP V5VH92
B	0	HIS	-	expression tag	UNP V5VH92

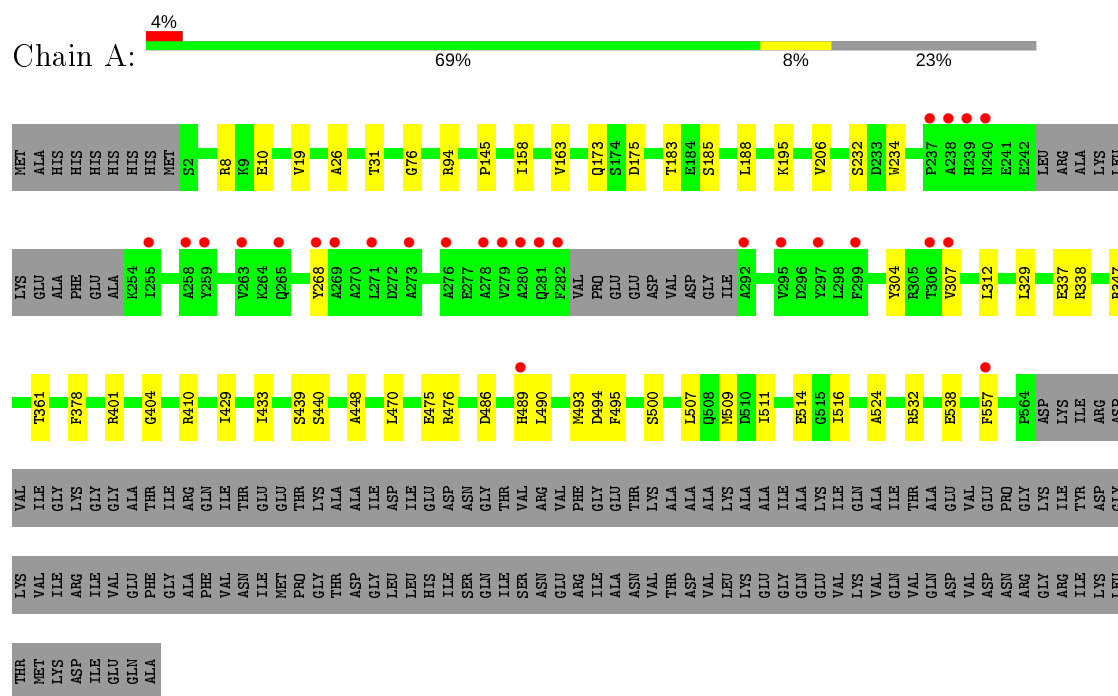
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	254	Total	O	0	1
			255	255		
2	B	250	Total	O	0	0
			250	250		

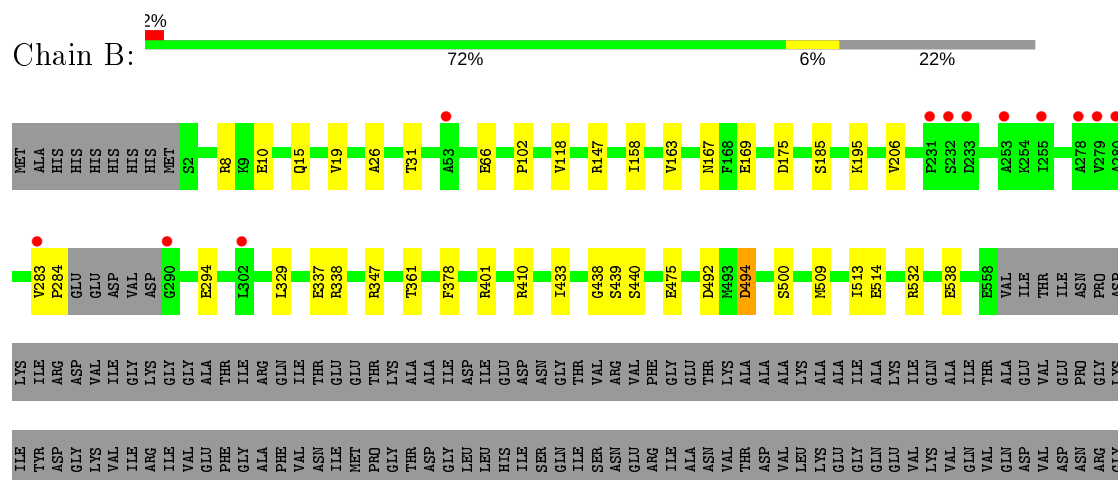
3 Residue-property plots [i](#)

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 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: Polyrribonucleotide nucleotidyltransferase



- Molecule 1: Polyrribonucleotide nucleotidyltransferase



ARG
ILE
LYS
LEU
THR
MET
LYS
ASP
ILE
GLU
GLN
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	93.69Å 93.69Å 266.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.44 – 2.50 46.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.44-2.50) 99.8 (46.85-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_3092)	Depositor
R, R_{free}	0.157 , 0.207 0.158 , 0.208	Depositor DCC
R_{free} test set	2020 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.129 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8614	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 3.44% 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	0.34	0/4071	0.54	0/5525
1	B	0.33	0/4175	0.55	0/5661
All	All	0.34	0/8246	0.54	0/11186

There are no bond length outliers.

There are no bond angle outliers.

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	4004	0	3911	33	0
1	B	4105	0	4047	26	0
2	A	255	0	0	4	0
2	B	250	0	0	6	0
All	All	8614	0	7958	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (59) 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:401:ARG:NH1	2:A:701:HOH:O	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:SER:O	1:A:532:ARG:NH2	2.17	0.77
1:A:347:ARG:NH1	2:A:704:HOH:O	2.18	0.77
1:A:486:ASP:O	1:A:489:HIS:ND1	2.21	0.73
1:B:329:LEU:HD12	1:B:538:GLU:HG3	1.73	0.71
1:B:8[B]:ARG:NH1	1:B:10:GLU:OE2	2.23	0.70
1:A:10:GLU:HG2	1:A:19:VAL:HG22	1.75	0.68
1:B:500:SER:O	1:B:532:ARG:NH2	2.30	0.64
1:B:494:ASP:OD2	2:B:701:HOH:O	2.15	0.63
1:A:329:LEU:HD12	1:A:538:GLU:HG3	1.81	0.62
1:A:470:LEU:HB3	1:A:493:MET:HB3	1.83	0.61
1:B:158:ILE:HD12	1:B:163:VAL:HG21	1.82	0.61
1:A:76:GLY:O	2:A:702:HOH:O	2.16	0.60
1:A:175:ASP:HA	1:A:195:LYS:HD2	1.83	0.60
1:B:175:ASP:HA	1:B:195:LYS:HD2	1.83	0.59
1:B:147:ARG:NH1	2:B:703:HOH:O	2.35	0.59
1:B:10:GLU:HG2	1:B:19:VAL:HG22	1.85	0.58
1:A:158:ILE:HD12	1:A:163:VAL:HG21	1.86	0.57
1:A:26:ALA:HB3	1:A:31:THR:HG21	1.86	0.57
1:A:401:ARG:NH1	1:A:401:ARG:HB3	2.21	0.56
1:A:94:ARG:HH11	1:A:404:GLY:HA3	1.69	0.55
1:A:304:TYR:CD2	1:A:490:LEU:HD22	2.42	0.55
1:A:94:ARG:NH1	1:A:404:GLY:HA3	2.22	0.54
1:B:347:ARG:NH1	2:B:707:HOH:O	2.38	0.52
1:A:307:VAL:HB	1:A:490:LEU:CD1	2.40	0.51
1:B:26:ALA:HB3	1:B:31:THR:HG21	1.93	0.51
1:B:15:GLN:HG2	2:B:831:HOH:O	2.11	0.51
1:B:433:ILE:HD12	1:B:440:SER:HB2	1.93	0.50
1:A:495:PHE:CZ	1:A:524:ALA:HB1	2.48	0.49
1:A:232:SER:OG	2:A:703:HOH:O	2.18	0.49
1:A:183:THR:HG23	1:A:188:LEU:HD11	1.94	0.49
1:B:401:ARG:HB3	1:B:401:ARG:NH2	2.28	0.49
1:A:433:ILE:HD12	1:A:440:SER:HB2	1.95	0.48
1:A:433:ILE:CD1	1:A:440:SER:HB2	2.44	0.48
1:A:185:SER:OG	1:A:514:GLU:OE1	2.21	0.48
1:B:185:SER:OG	1:B:514:GLU:OE2	2.14	0.47
1:B:492:ASP:HB3	1:B:513:ILE:HG12	1.97	0.47
1:A:206:VAL:HG21	1:A:509:MET:HE3	1.97	0.46
1:B:433:ILE:CD1	1:B:440:SER:HB2	2.44	0.46
1:B:66:GLU:HG2	1:B:118:VAL:HG21	1.98	0.45
1:A:429:ILE:HD13	1:A:448:ALA:HB1	1.98	0.45
1:B:378:PHE:CE2	1:B:410:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:HA	1:A:489:HIS:HD1	1.83	0.44
1:B:102:PRO:HG3	2:B:879:HOH:O	2.18	0.44
1:B:338:ARG:HD3	1:B:338:ARG:HA	1.78	0.44
1:A:507:LEU:HD21	1:A:509:MET:HE1	1.99	0.44
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.80	0.43
1:B:167:ASN:OD1	1:B:169:GLU:HG3	2.18	0.43
1:B:347:ARG:NH2	1:B:438:GLY:O	2.52	0.43
1:B:283:VAL:HA	1:B:284:PRO:HD2	1.84	0.42
1:A:268:TYR:OH	1:A:486:ASP:OD1	2.17	0.42
1:A:511:ILE:HG23	1:A:516:ILE:HD12	2.02	0.42
1:B:206:VAL:HG21	1:B:509:MET:HE3	2.01	0.42
1:A:489:HIS:CE1	1:A:490:LEU:HG	2.55	0.41
1:A:338:ARG:HA	1:A:338:ARG:HD3	1.76	0.41
1:B:514:GLU:HG3	2:B:836:HOH:O	2.20	0.41
1:A:145:PRO:HG3	1:A:234:TRP:HB3	2.02	0.41
1:A:378:PHE:CE1	1:A:410:ARG:HG3	2.56	0.41
1:B:401:ARG:CZ	1:B:401:ARG:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	539/705 (76%)	529 (98%)	9 (2%)	1 (0%)	47	68
1	B	550/705 (78%)	536 (98%)	13 (2%)	1 (0%)	47	68
All	All	1089/1410 (77%)	1065 (98%)	22 (2%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	SER

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Mol	Chain	Res	Type
1	B	439	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/558 (72%)	393 (98%)	9 (2%)	52	77
1	B	415/558 (74%)	410 (99%)	5 (1%)	71	88
All	All	817/1116 (73%)	803 (98%)	14 (2%)	62	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8[A]	ARG
1	A	8[B]	ARG
1	A	173	GLN
1	A	337	GLU
1	A	361	THR
1	A	475	GLU
1	A	476	ARG
1	A	494	ASP
1	A	557	PHE
1	B	294	GLU
1	B	337	GLU
1	B	361	THR
1	B	475	GLU
1	B	494	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	405	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](#)

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	543/705 (77%)	-0.19	27 (4%)	28 30	23, 39, 88, 129	0
1	B	552/705 (78%)	-0.20	12 (2%)	62 65	24, 41, 80, 127	0
All	All	1095/1410 (77%)	-0.20	39 (3%)	42 46	23, 40, 87, 129	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	ASP	5.7
1	A	280	ALA	5.4
1	A	255	ILE	4.8
1	A	268	TYR	4.2
1	A	489	HIS	4.1
1	B	280	ALA	4.1
1	A	269	ALA	4.0
1	A	276	ALA	3.9
1	A	297	TYR	3.9
1	A	237	PRO	3.8
1	B	231	PRO	3.6
1	A	279	VAL	3.6
1	B	283	VAL	3.5
1	A	282	PHE	3.4
1	B	279	VAL	3.4
1	A	259	TYR	3.4
1	A	273	ALA	3.3
1	A	238	ALA	3.3
1	A	239	HIS	3.2
1	A	263	VAL	3.1
1	A	278	ALA	3.1
1	A	292	ALA	3.1
1	A	265	GLN	3.0
1	B	53	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	2.9
1	B	232	SER	2.8
1	A	240	ASN	2.7
1	B	302	LEU	2.7
1	A	306	THR	2.7
1	A	557	PHE	2.7
1	A	258	ALA	2.5
1	A	299	PHE	2.5
1	B	278	ALA	2.3
1	B	253	ALA	2.3
1	A	281	GLN	2.3
1	B	255	ILE	2.2
1	A	271	LEU	2.2
1	A	295	VAL	2.1
1	A	307	VAL	2.1

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 carbohydrates 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.