



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:52 PM GMT

PDB ID : 1R0V
Title : Structure Determination of the Dimeric Endonuclease in a Pseudo-face-centered P21212 space group
Authors : Li, H.; Zhang, Y.
Deposited on : 2003-09-23
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

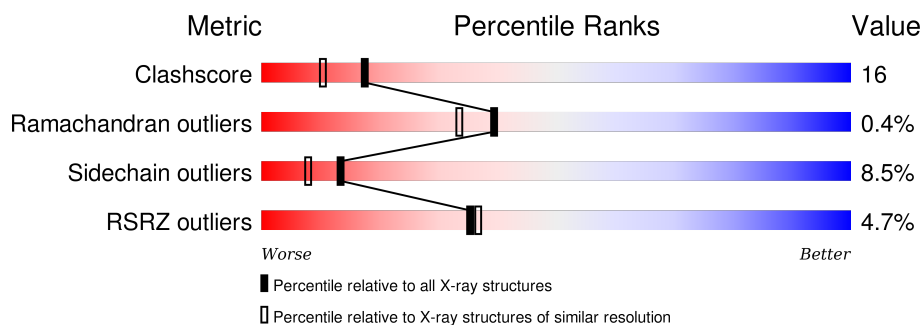
1 Overall quality at a glance

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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	305	<div> <div>4%</div> <div> <div>42%</div> <div>30%</div> <div>6%</div> <div>•</div> <div>20%</div> </div> </div>
1	B	305	<div> <div>4%</div> <div> <div>37%</div> <div>31%</div> <div>9%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	305	<div> <div>3%</div> <div> <div>43%</div> <div>28%</div> <div>7%</div> <div>•</div> <div>20%</div> </div> </div>
1	D	305	<div> <div>4%</div> <div> <div>46%</div> <div>26%</div> <div>7%</div> <div>•</div> <div>20%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9073 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 tRNA-intron endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			2050	1309	351	385	5			
1	B	244	Total	C	N	O	S	0	0	0
			2050	1309	351	385	5			
1	C	244	Total	C	N	O	S	0	0	0
			2050	1309	351	385	5			
1	D	243	Total	C	N	O	S	0	0	0
			2042	1305	350	382	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	VAL	ILE	CONFLICT	UNP O29362
B	152	VAL	ILE	CONFLICT	UNP O29362
C	152	VAL	ILE	CONFLICT	UNP O29362
D	152	VAL	ILE	CONFLICT	UNP O29362

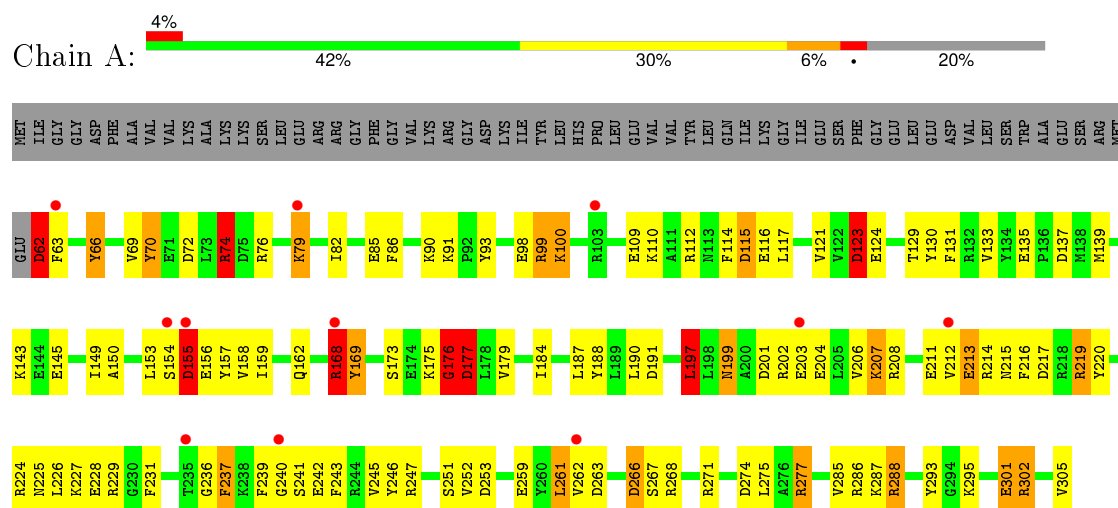
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	232	Total	O	0	0
			232	232		
2	B	215	Total	O	0	0
			215	215		
2	C	199	Total	O	0	0
			199	199		
2	D	235	Total	O	0	0
			235	235		

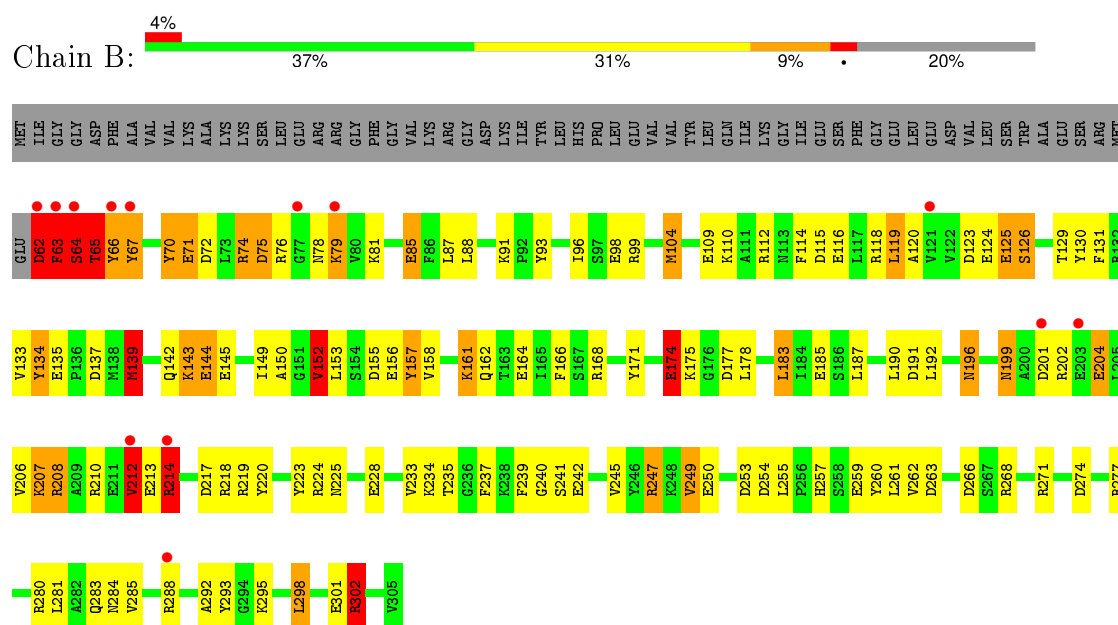
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

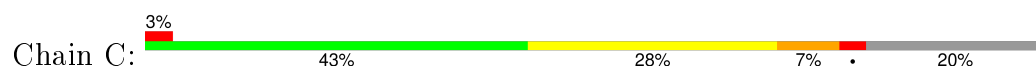
- Molecule 1: tRNA-intron endonuclease

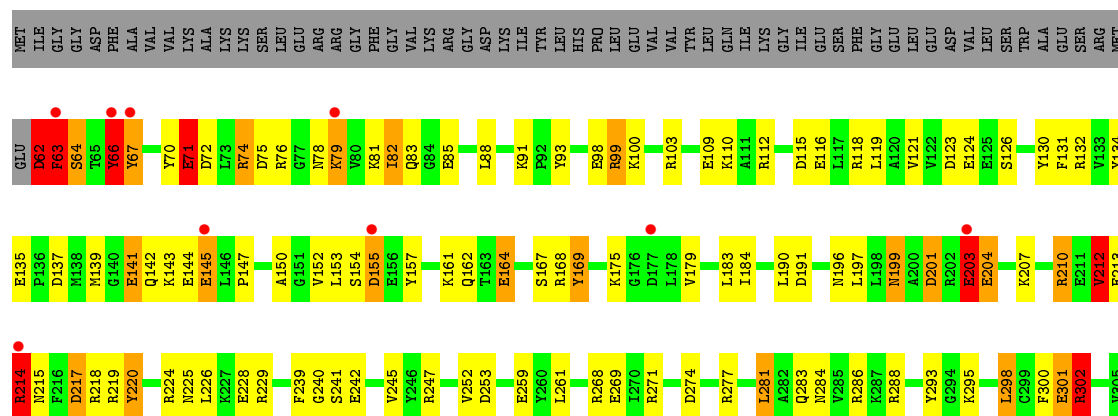


- Molecule 1: tRNA-intron endonuclease



- Molecule 1: tRNA-intron endonuclease

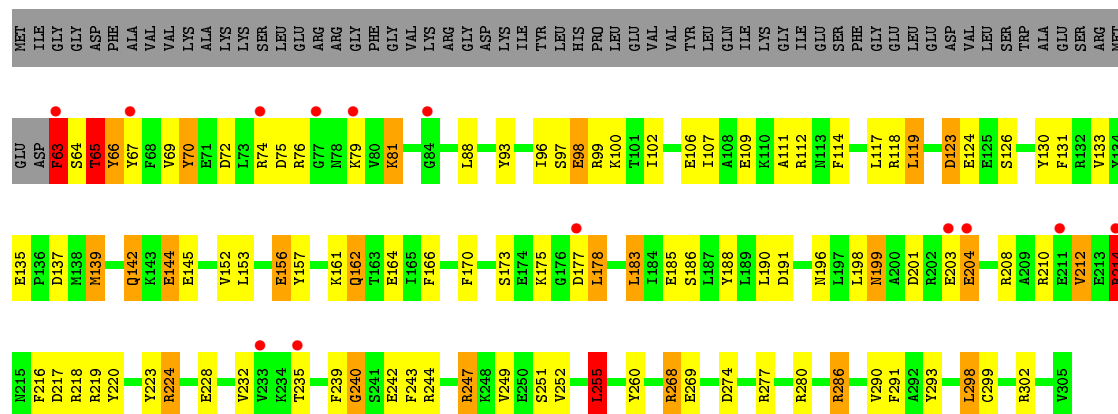




• Molecule 1: tRNA-intron endonuclease



Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	128.12Å 144.15Å 52.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.35 – 2.00 28.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (95.35-2.00) 87.2 (28.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.242 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 70265 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9073	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.05 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4528e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.94	52/2085 (2.5%)	1.77	63/2798 (2.3%)
1	B	2.30	106/2085 (5.1%)	2.20	116/2798 (4.1%)
1	C	2.27	86/2085 (4.1%)	2.22	97/2798 (3.5%)
1	D	2.00	56/2077 (2.7%)	1.85	58/2787 (2.1%)
All	All	2.13	300/8332 (3.6%)	2.02	334/11181 (3.0%)

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
1	B	0	4
1	C	0	1
1	D	0	1
All	All	0	6

The worst 5 of 300 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	124	GLU	CD-OE2	-13.79	1.10	1.25
1	B	144	GLU	CD-OE2	-12.54	1.11	1.25
1	A	157	TYR	CE1-CZ	-12.37	1.22	1.38
1	B	63	PHE	CB-CG	-12.15	1.30	1.51
1	C	70	TYR	CE2-CZ	-12.14	1.22	1.38

The worst 5 of 334 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	ARG	NE-CZ-NH1	32.39	136.50	120.30
1	C	268	ARG	NE-CZ-NH2	-24.40	108.10	120.30
1	D	268	ARG	NE-CZ-NH1	21.44	131.02	120.30
1	B	63	PHE	N-CA-C	-19.17	59.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	PHE	C-N-CA	-19.16	73.79	121.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	62	ASP	Mainchain,Peptide
1	B	63	PHE	Mainchain,Peptide
1	C	63	PHE	Peptide
1	D	63	PHE	Peptide

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	2050	0	2055	82	1
1	B	2050	0	2054	89	2
1	C	2050	0	2054	74	3
1	D	2042	0	2051	62	3
2	A	232	0	0	22	2
2	B	215	0	0	25	1
2	C	199	0	0	30	1
2	D	235	0	0	21	1
All	All	9073	0	8214	262	7

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 16.

The worst 5 of 262 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:D:139:MET:CE	1:D:139:MET:SD	2.03	1.46
1:B:104:MET:CE	1:B:104:MET:SD	2.06	1.40
1:B:175:LYS:HG2	2:B:492:HOH:O	1.12	1.26
1:B:175:LYS:HB2	2:B:506:HOH:O	1.13	1.26
1:D:175:LYS:HG2	2:D:526:HOH:O	1.34	1.22

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:NE	1:C:203:GLU:OE1[3_545]	1.97	0.23
1:D:224:ARG:NH2	2:A:413:HOH:O[3_556]	1.99	0.21
1:A:203:GLU:OE2	1:D:224:ARG:NH2[3_546]	2.06	0.14
1:C:210:ARG:NH2	2:B:517:HOH:O[3_555]	2.07	0.13
1:D:269:GLU:OE2	2:A:529:HOH:O[3_556]	2.13	0.07

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	242/305 (79%)	233 (96%)	6 (2%)	3 (1%)	16	8
1	B	242/305 (79%)	233 (96%)	9 (4%)	0	100	100
1	C	242/305 (79%)	234 (97%)	7 (3%)	1 (0%)	39	33
1	D	241/305 (79%)	234 (97%)	7 (3%)	0	100	100
All	All	967/1220 (79%)	934 (97%)	29 (3%)	4 (0%)	39	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLY
1	A	177	ASP
1	A	155	ASP
1	C	155	ASP

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	222/273 (81%)	206 (93%)	16 (7%)	18	12
1	B	222/273 (81%)	202 (91%)	20 (9%)	12	7
1	C	222/273 (81%)	201 (90%)	21 (10%)	11	6
1	D	221/273 (81%)	203 (92%)	18 (8%)	15	9
All	All	887/1092 (81%)	812 (92%)	75 (8%)	13	8

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	LYS
1	C	82	ILE
1	D	203	GLU
1	B	298	LEU
1	C	71	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	142	GLN
1	B	162	GLN
1	C	284	ASN
1	A	257	HIS
1	D	142	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	244/305 (80%)	0.09	11 (4%) 37 38	19, 27, 38, 50	0
1	B	244/305 (80%)	0.17	13 (5%) 30 32	19, 27, 38, 52	0
1	C	244/305 (80%)	0.12	9 (3%) 45 47	19, 27, 39, 50	0
1	D	243/305 (79%)	0.10	13 (5%) 30 32	18, 27, 38, 51	0
All	All	975/1220 (79%)	0.12	46 (4%) 35 37	18, 27, 39, 52	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	PHE	14.6
1	B	63	PHE	9.3
1	D	63	PHE	6.0
1	C	67	TYR	4.6
1	B	67	TYR	4.5

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.