



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:37 PM GMT

PDB ID : 4IWG  
Title : Crystal Structure of the Conserved Hypothetical Protein MJ0927 from Methanocaldococcus jannaschii (in C2221 form)  
Authors : Kuan, S.M.; Chen, S.C.; Yang, C.S.; Chen, Y.R.; Liu, Y.H.; Chen, Y.  
Deposited on : 2013-01-23  
Resolution : 2.47 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](mailto: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.

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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

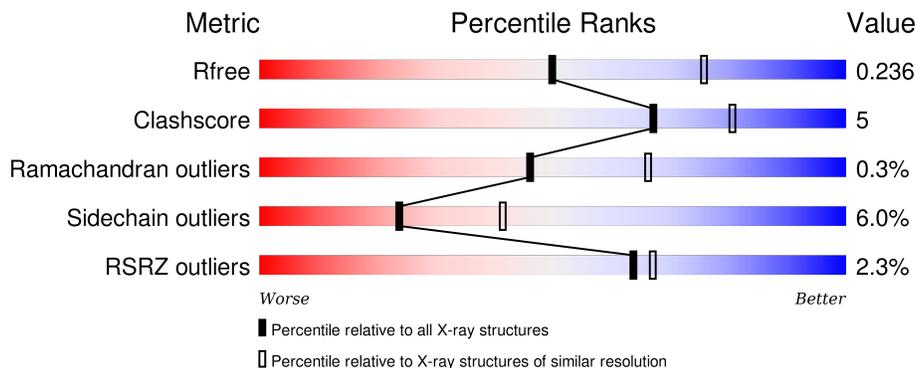
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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))
$R_{free}$	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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  $\geq 3$ , 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	252	 81% 14% . .
1	B	252	 81% 13% . .
1	C	252	 83% 12% . .

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5922 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 UPF0135 protein MJ0927.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	1932	1255	307	367	3	0	0	0
1	B	244	1932	1255	307	367	3	0	0	0
1	C	244	1932	1255	307	367	3	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	LEU	-	EXPRESSION TAG	UNP Q58337
A	251	GLU	-	EXPRESSION TAG	UNP Q58337
A	252	HIS	-	EXPRESSION TAG	UNP Q58337
A	253	HIS	-	EXPRESSION TAG	UNP Q58337
A	254	HIS	-	EXPRESSION TAG	UNP Q58337
A	255	HIS	-	EXPRESSION TAG	UNP Q58337
A	256	HIS	-	EXPRESSION TAG	UNP Q58337
A	257	HIS	-	EXPRESSION TAG	UNP Q58337
B	250	LEU	-	EXPRESSION TAG	UNP Q58337
B	251	GLU	-	EXPRESSION TAG	UNP Q58337
B	252	HIS	-	EXPRESSION TAG	UNP Q58337
B	253	HIS	-	EXPRESSION TAG	UNP Q58337
B	254	HIS	-	EXPRESSION TAG	UNP Q58337
B	255	HIS	-	EXPRESSION TAG	UNP Q58337
B	256	HIS	-	EXPRESSION TAG	UNP Q58337
B	257	HIS	-	EXPRESSION TAG	UNP Q58337
C	250	LEU	-	EXPRESSION TAG	UNP Q58337
C	251	GLU	-	EXPRESSION TAG	UNP Q58337
C	252	HIS	-	EXPRESSION TAG	UNP Q58337
C	253	HIS	-	EXPRESSION TAG	UNP Q58337
C	254	HIS	-	EXPRESSION TAG	UNP Q58337
C	255	HIS	-	EXPRESSION TAG	UNP Q58337
C	256	HIS	-	EXPRESSION TAG	UNP Q58337

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Chain	Residue	Modelled	Actual	Comment	Reference
C	257	HIS	-	EXPRESSION TAG	UNP Q58337

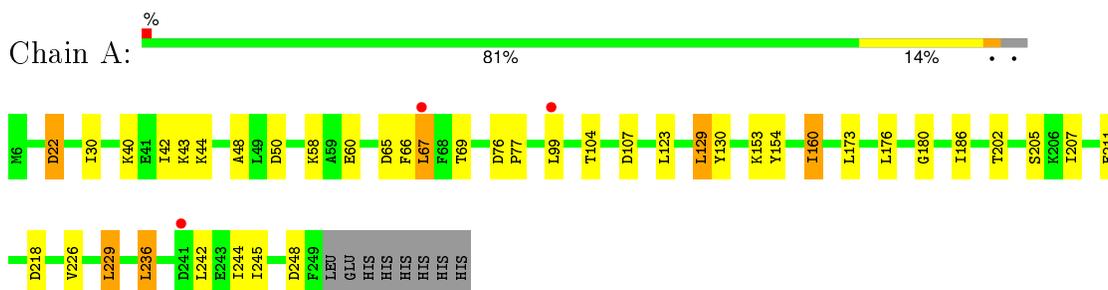
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	43	Total O 43 43	0	0
2	B	48	Total O 48 48	0	0
2	C	35	Total O 35 35	0	0

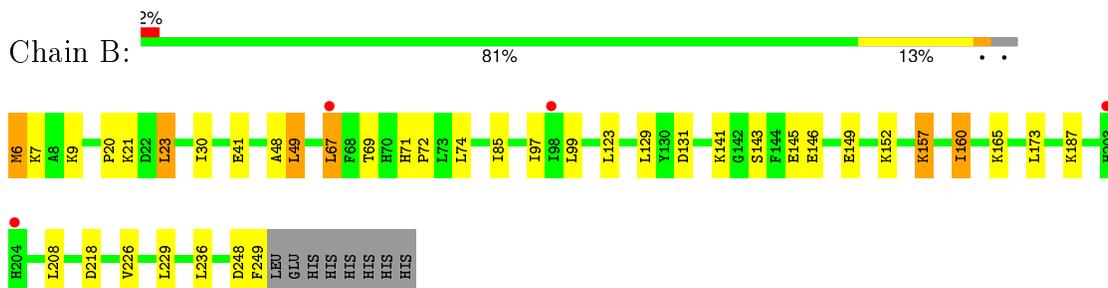
### 3 Residue-property plots [i](#)

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

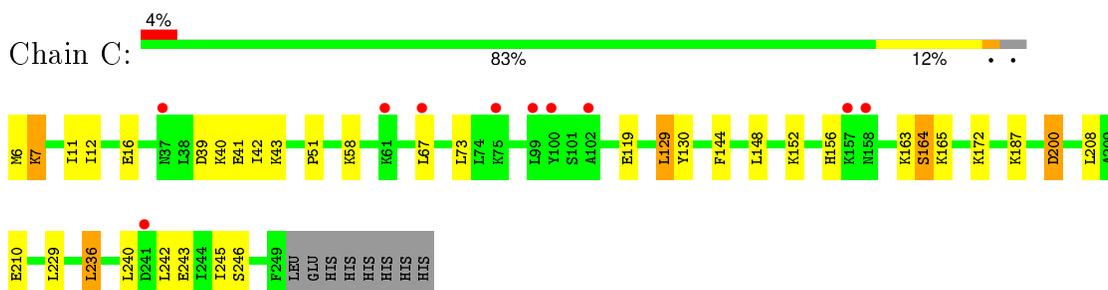
- Molecule 1: UPF0135 protein MJ0927



- Molecule 1: UPF0135 protein MJ0927



- Molecule 1: UPF0135 protein MJ0927



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.21Å 172.94Å 147.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.47 24.98 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.98-2.47) 99.9 (24.98-2.47)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 2.47Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.181 , 0.237 0.179 , 0.236	Depositor DCC
$R_{free}$ test set	1870 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.3	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 37422 reflections	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	0.39	0/1967	0.54	0/2651
1	B	0.40	0/1967	0.55	0/2651
1	C	0.38	0/1967	0.55	0/2651
All	All	0.39	0/5901	0.55	0/7953

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 [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	1932	0	1978	19	0
1	B	1932	0	1978	21	0
1	C	1932	0	1978	16	0
2	A	43	0	0	1	0
2	B	48	0	0	3	0
2	C	35	0	0	1	0
All	All	5922	0	5934	56	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 (56) 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:187:LYS:O	2:B:336:HOH:O	2.04	0.73
1:A:22:ASP:OD1	2:A:334:HOH:O	2.09	0.69
1:C:200:ASP:OD1	2:C:330:HOH:O	2.10	0.69
1:A:160:ILE:HG23	1:A:218:ASP:HB3	1.76	0.67
1:B:49:LEU:HD12	1:B:229:LEU:HD12	1.80	0.64
1:B:97:ILE:O	2:B:327:HOH:O	2.14	0.64
1:C:242:LEU:O	1:C:243:GLU:HB3	2.01	0.61
1:B:131:ASP:OD1	2:B:324:HOH:O	2.17	0.58
1:A:40:LYS:HE3	1:A:65:ASP:HB2	1.85	0.58
1:B:123:LEU:HD21	1:B:173:LEU:HD23	1.86	0.58
1:A:123:LEU:HD21	1:A:173:LEU:HD23	1.87	0.57
1:B:187:LYS:HG3	1:B:208:LEU:HD21	1.91	0.53
1:A:44:LYS:HE2	1:A:245:ILE:HD13	1.92	0.52
1:B:143:SER:OG	1:B:146:GLU:HG3	2.09	0.52
1:C:164:SER:HB3	1:C:210:GLU:HA	1.92	0.51
1:B:20:PRO:HD2	1:B:23:LEU:HD22	1.91	0.51
1:C:6:MET:HE1	1:C:240:LEU:HB3	1.94	0.50
1:C:144:PHE:CE2	1:C:163:LYS:HE2	2.47	0.49
1:B:248:ASP:HB3	1:B:249:PHE:HD1	1.78	0.48
1:B:21:LYS:HD2	1:B:30:ILE:HD13	1.95	0.48
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.73	0.48
1:C:7:LYS:H	1:C:41:GLU:HA	1.80	0.47
1:A:236:LEU:HB3	1:A:244:ILE:HD13	1.97	0.47
1:C:187:LYS:HG3	1:C:208:LEU:HD21	1.97	0.47
1:B:6:MET:O	1:B:7:LYS:HB3	2.15	0.46
1:C:11:ILE:HD11	1:C:242:LEU:HD11	1.96	0.46
1:A:42:ILE:HD12	1:A:66:PHE:HB2	1.98	0.46
1:C:129:LEU:HD13	1:C:130:TYR:CE2	2.51	0.46
1:C:7:LYS:HG2	1:C:39:ASP:O	2.16	0.45
1:B:6:MET:N	1:B:41:GLU:OE2	2.50	0.45
1:A:153:LYS:HD3	1:A:154:TYR:CE2	2.52	0.45
1:B:141:LYS:HE3	1:B:141:LYS:HB3	1.79	0.45
1:C:6:MET:O	1:C:7:LYS:HB2	2.16	0.44
1:B:74:LEU:HD21	1:B:85:ILE:HD13	2.00	0.44
1:B:7:LYS:HD3	1:B:9:LYS:HE2	2.00	0.44
1:A:129:LEU:HD13	1:A:130:TYR:CE2	2.53	0.44
1:A:76:ASP:HA	1:A:77:PRO:HD3	1.92	0.43
1:A:176:LEU:HD12	1:A:180:GLY:HA3	2.00	0.43
1:A:48:ALA:O	1:A:69:THR:HA	2.18	0.43
1:C:51:PRO:HG2	1:C:73:LEU:HA	2.01	0.43
1:A:67:LEU:HD13	1:A:99:LEU:HD13	2.00	0.42
1:A:186:ILE:HD12	1:A:205:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:HA	1:C:156:HIS:O	2.20	0.42
1:B:160:ILE:HG23	1:B:218:ASP:HB3	2.02	0.41
1:B:71:HIS:HA	1:B:72:PRO:HD3	1.86	0.41
1:B:67:LEU:HD13	1:B:99:LEU:HD13	2.01	0.41
1:C:148:LEU:HA	1:C:148:LEU:HD23	1.96	0.41
1:A:30:ILE:HG13	1:A:30:ILE:H	1.77	0.41
1:A:207:ILE:O	1:A:211:GLU:HG2	2.20	0.41
1:A:104:THR:HA	1:A:107:ASP:OD2	2.21	0.41
1:C:236:LEU:HA	1:C:236:LEU:HD12	1.87	0.40
1:B:152:LYS:O	1:B:157:LYS:HD2	2.21	0.40
1:C:12:ILE:O	1:C:16:GLU:HG3	2.22	0.40
1:A:43:LYS:HE3	1:A:43:LYS:HB2	1.86	0.40
1:B:229:LEU:HA	1:B:229:LEU:HD23	1.79	0.40
1:B:48:ALA:O	1:B:69:THR:HA	2.21	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	242/252 (96%)	236 (98%)	6 (2%)	0	100	100
1	B	242/252 (96%)	233 (96%)	9 (4%)	0	100	100
1	C	242/252 (96%)	225 (93%)	15 (6%)	2 (1%)	24	39
All	All	726/756 (96%)	694 (96%)	30 (4%)	2 (0%)	46	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	200	ASP
1	C	7	LYS

### 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	215/223 (96%)	202 (94%)	13 (6%)	24	41
1	B	215/223 (96%)	203 (94%)	12 (6%)	26	45
1	C	215/223 (96%)	201 (94%)	14 (6%)	21	37
All	All	645/669 (96%)	606 (94%)	39 (6%)	24	41

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	50	ASP
1	A	58	LYS
1	A	60	GLU
1	A	67	LEU
1	A	129	LEU
1	A	160	ILE
1	A	202	THR
1	A	226	VAL
1	A	229	LEU
1	A	236	LEU
1	A	242	LEU
1	A	248	ASP
1	B	6	MET
1	B	23	LEU
1	B	49	LEU
1	B	67	LEU
1	B	129	LEU
1	B	145	GLU
1	B	149	GLU
1	B	157	LYS
1	B	160	ILE
1	B	165	LYS
1	B	226	VAL
1	B	236	LEU
1	C	40	LYS

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Mol	Chain	Res	Type
1	C	42	ILE
1	C	43	LYS
1	C	58	LYS
1	C	67	LEU
1	C	119	GLU
1	C	129	LEU
1	C	164	SER
1	C	165	LYS
1	C	172	LYS
1	C	229	LEU
1	C	236	LEU
1	C	245	ILE
1	C	246	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	244/252 (96%)	-0.21	3 (1%) 81 83	31, 44, 62, 76	0
1	B	244/252 (96%)	-0.24	4 (1%) 74 77	33, 46, 61, 72	0
1	C	244/252 (96%)	-0.07	10 (4%) 41 45	34, 50, 75, 90	0
All	All	732/756 (96%)	-0.17	17 (2%) 64 67	31, 46, 69, 90	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	LYS	3.3
1	B	67	LEU	2.9
1	A	99	LEU	2.7
1	C	158	ASN	2.7
1	A	67	LEU	2.5
1	C	99	LEU	2.4
1	A	241	ASP	2.3
1	B	203	HIS	2.3
1	C	241	ASP	2.3
1	C	37	ASN	2.2
1	C	67	LEU	2.2
1	B	98	ILE	2.1
1	B	204	HIS	2.1
1	C	75	LYS	2.1
1	C	102	ALA	2.1
1	C	157	LYS	2.0
1	C	100	TYR	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

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.