



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 AM GMT

PDB ID : 3F1L  
Title : The 0.95 Å structure of an oxidoreductase, yciK from E.coli  
Authors : Vijayalakshmi, J.; Woodard, R.W.  
Deposited on : 2008-10-28  
Resolution : 0.95 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

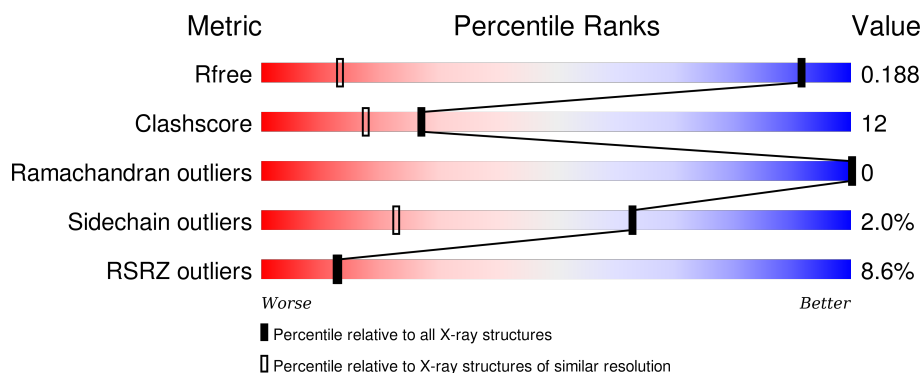
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 0.95 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	1319 (1.10-0.82)
Clashscore	102246	1031 (1.08-0.84)
Ramachandran outliers	100387	1331 (1.10-0.82)
Sidechain outliers	100360	1330 (1.10-0.82)
RSRZ outliers	91569	1324 (1.10-0.82)

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	<div> <div>8%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	B	252	<div> <div>9%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8370 atoms, of which 3767 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 Uncharacterized oxidoreductase yciK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	H	N	O	S	24	5	0
			3807	1201	1885	345	361	15			
1	B	244	Total	C	H	N	O	S	0	5	0
			3800	1197	1882	342	363	16			

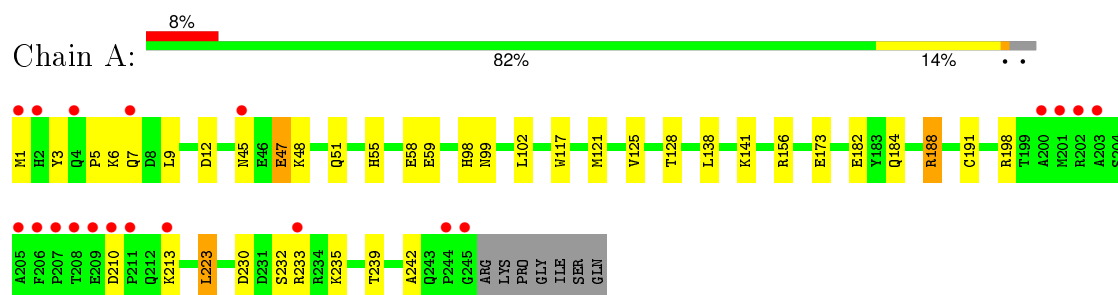
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	403	Total	O	0	0
			403	403		
2	B	360	Total	O	0	0
			360	360		

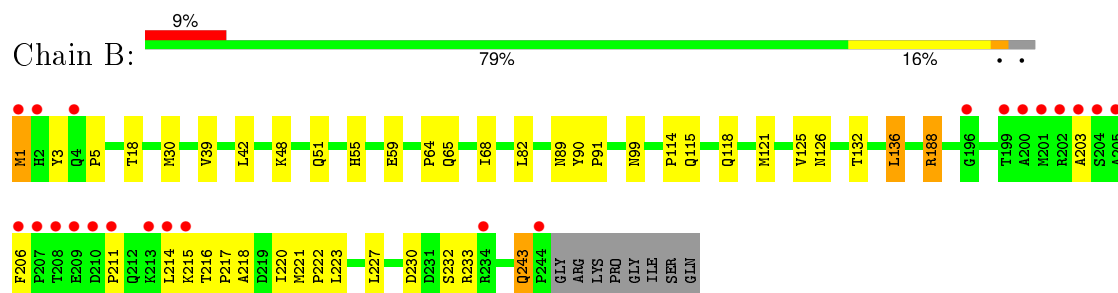
### 3 Residue-property plots

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: Uncharacterized oxidoreductase yciK



- Molecule 1: Uncharacterized oxidoreductase yciK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.87Å 66.80Å 65.05Å 90.00° 109.03° 90.00°	Depositor
Resolution (Å)	34.14 – 0.95 34.14 – 0.90	Depositor EDS
% Data completeness (in resolution range)	86.7 (34.14-0.95) 80.6 (34.14-0.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 0.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.171 , 0.192 0.166 , 0.188	Depositor DCC
$R_{free}$ test set	1822 reflections (0.77%)	DCC
Wilson B-factor (Å <sup>2</sup> )	8.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 258779 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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 25.05 % 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 3.4122e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0/1973	0.69	2/2673 (0.1%)
1	B	0.36	0/1973	0.62	2/2674 (0.1%)
All	All	0.38	0/3946	0.65	4/5347 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	A	188	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	188	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	188	ARG	NE-CZ-NH2	-6.99	116.80	120.30

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	1922	1885	1902	53	0
1	B	1918	1882	1901	46	0
2	A	403	0	0	19	0
2	B	360	0	0	13	0
All	All	4603	3767	3803	92	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 12.

All (92) 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:132:THR:O	1:B:136:LEU:HD13	1.51	1.08
1:A:156:ARG:HH21	1:A:239:THR:HG22	1.22	1.00
1:A:121:MET:HE2	1:B:121:MET:HE2	1.54	0.89
1:A:173:GLU:OE2	1:A:239:THR:HG21	1.75	0.87
1:A:191:CYS:HB2	1:A:239:THR:HG23	1.54	0.87
1:B:48:LYS:O	1:B:51:GLN:HG2	1.79	0.83
1:A:121:MET:HE2	1:B:121:MET:CE	2.10	0.82
1:B:1:MET:HE1	1:B:223:LEU:HD13	1.63	0.80
1:A:3:TYR:CE1	1:A:5:PRO:HG3	2.19	0.78
1:A:128:THR:O	2:A:700:HOH:O	2.01	0.77
1:A:182:GLU:HB3	2:A:724:HOH:O	1.85	0.76
1:A:230:ASP:O	1:A:233[A]:ARG:HG2	1.87	0.75
1:A:128:THR:HG23	2:A:700:HOH:O	1.87	0.74
1:A:184:GLN:HG3	2:A:356:HOH:O	1.88	0.72
1:B:211:PRO:HA	1:B:214:LEU:HD23	1.71	0.71
1:A:98:HIS:NE2	2:A:700:HOH:O	2.22	0.71
1:A:121:MET:CE	1:B:121:MET:HE2	2.20	0.71
1:A:188:ARG:HD3	1:A:232:SER:O	1.90	0.71
1:A:98:HIS:CE1	2:A:700:HOH:O	2.46	0.69
1:A:210:ASP:HB3	1:A:213:LYS:HE2	1.76	0.68
1:B:1:MET:CE	1:B:223:LEU:HD13	2.24	0.68
1:B:3:TYR:CE1	1:B:5:PRO:HG3	2.29	0.68
1:A:156:ARG:HH21	1:A:239:THR:CG2	2.03	0.65
1:A:121:MET:CE	1:B:121:MET:CE	2.75	0.65
1:B:30[A]:MET:HE2	2:B:348:HOH:O	1.96	0.65
1:B:216:THR:HG22	1:B:218:ALA:H	1.61	0.65
1:A:128:THR:CG2	2:A:700:HOH:O	2.44	0.64
1:B:42:LEU:HD21	1:B:82:LEU:HD21	1.80	0.63
1:B:114:PRO:O	1:B:118:GLN:HG3	1.98	0.63
1:B:30[A]:MET:HB3	2:B:348:HOH:O	2.01	0.61
1:A:173:GLU:OE1	1:A:239:THR:OG1	2.18	0.61
1:A:233[A]:ARG:HG3	2:A:298:HOH:O	2.00	0.60
1:B:59:GLU:OE1	2:B:348:HOH:O	2.17	0.60
1:A:55:HIS:O	1:A:58:GLU:HG2	2.02	0.60
1:A:223:LEU:HD12	1:A:242:ALA:HA	1.84	0.59
1:A:156:ARG:NH2	1:A:239:THR:HG22	2.06	0.58
1:B:132:THR:HG22	1:B:136:LEU:HD11	1.85	0.58
1:B:216:THR:HG23	1:B:217:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG22	1:B:243:GLN:HG2	1.87	0.57
1:B:1:MET:SD	1:B:223:LEU:HA	2.44	0.57
1:A:121:MET:HE1	1:A:125:VAL:HG21	1.88	0.55
1:B:206:PHE:CD2	2:B:755:HOH:O	2.53	0.55
1:B:99[B]:ASN:OD1	2:B:352:HOH:O	2.18	0.54
1:B:65:GLN:HE22	1:B:89:ASN:HD22	1.55	0.54
1:A:102[B]:LEU:HD21	2:A:547:HOH:O	2.07	0.53
1:B:1:MET:HB2	1:B:3:TYR:HB2	1.89	0.53
1:A:3:TYR:CD1	1:A:5:PRO:HG3	2.43	0.53
1:A:7:GLN:O	1:A:7:GLN:HG3	2.08	0.53
1:B:1:MET:N	2:B:762:HOH:O	2.42	0.53
1:B:55:HIS:CD2	2:B:664:HOH:O	2.62	0.53
1:A:121:MET:HG3	1:B:126:ASN:HD21	1.75	0.52
1:B:1:MET:HE3	1:B:223:LEU:HB2	1.90	0.52
1:A:1:MET:HG3	1:A:3:TYR:HB2	1.91	0.51
1:A:121:MET:CE	1:A:125:VAL:HG21	2.41	0.51
1:B:30[B]:MET:HB3	2:B:348:HOH:O	2.11	0.50
1:A:58:GLU:HB2	2:A:613:HOH:O	2.13	0.49
1:A:12:ASP:HB3	2:A:561:HOH:O	2.11	0.49
1:A:99:ASN:ND2	2:A:451:HOH:O	2.47	0.48
1:A:138:LEU:HD23	1:A:141[B]:LYS:CE	2.43	0.48
1:A:45:ASN:HB3	1:A:47[A]:GLU:OE1	2.14	0.48
1:A:117:TRP:HE1	1:B:126:ASN:HD22	1.62	0.47
2:A:434:HOH:O	1:B:114:PRO:HG3	2.15	0.47
1:A:138:LEU:HA	1:A:141[B]:LYS:NZ	2.30	0.47
1:A:98:HIS:HD2	2:A:300:HOH:O	1.97	0.47
1:B:115:GLN:HG3	2:B:713:HOH:O	2.15	0.47
1:A:188:ARG:HG2	1:A:235:LYS:O	2.15	0.46
1:B:132:THR:CG2	1:B:136:LEU:HD11	2.46	0.46
1:A:6:LYS:HE3	1:A:9:LEU:HA	1.98	0.46
1:A:156:ARG:HE	1:A:239:THR:HG21	1.82	0.45
1:B:18:THR:O	1:B:99[B]:ASN:HB3	2.16	0.44
1:B:206:PHE:CE2	2:B:755:HOH:O	2.71	0.44
1:B:68:ILE:HD12	1:B:68:ILE:N	2.33	0.44
1:B:188:ARG:HD3	1:B:232:SER:O	2.18	0.44
1:A:51:GLN:NE2	2:A:678:HOH:O	2.50	0.44
1:B:39:VAL:HG23	1:B:64:PRO:HB3	1.99	0.44
1:B:121:MET:CE	1:B:125:VAL:HG21	2.49	0.42
1:A:223:LEU:HD12	1:A:242:ALA:CA	2.48	0.42
1:A:48:LYS:HA	2:A:678:HOH:O	2.18	0.42
1:A:98:HIS:CD2	2:A:700:HOH:O	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASP:HA	1:B:233:ARG:HG3	2.01	0.41
1:A:55:HIS:O	1:A:59:GLU:HG2	2.20	0.41
1:B:230:ASP:HB3	2:B:527:HOH:O	2.20	0.41
1:B:221:MET:N	1:B:222:PRO:CD	2.84	0.41
1:A:138:LEU:HA	1:A:141[B]:LYS:HZ3	1.85	0.41
1:B:90:TYR:HA	1:B:91:PRO:HD3	1.93	0.41
1:B:203:ALA:HB3	2:B:304:HOH:O	2.20	0.41
1:A:121:MET:CE	1:B:121:MET:HE1	2.50	0.41
1:A:233[B]:ARG:HD3	2:A:410:HOH:O	2.20	0.40
1:A:58:GLU:CB	2:A:613:HOH:O	2.69	0.40
1:B:118:GLN:NE2	2:B:520:HOH:O	2.53	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	247/252 (98%)	240 (97%)	7 (3%)	0	100	100
1	B	247/252 (98%)	238 (96%)	9 (4%)	0	100	100
All	All	494/504 (98%)	478 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	207/209 (99%)	203 (98%)	4 (2%)	65	25
1	B	208/209 (100%)	203 (98%)	5 (2%)	57	16
All	All	415/418 (99%)	406 (98%)	9 (2%)	63	19

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47[A]	GLU
1	A	47[B]	GLU
1	A	198	ARG
1	A	223	LEU
1	B	1	MET
1	B	136	LEU
1	B	215	LYS
1	B	227	LEU
1	B	243	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	45	ASN
1	A	81	GLN
1	A	84	GLN
1	A	98	HIS
1	A	99	ASN
1	A	185	GLN
1	B	65	GLN
1	B	112	GLN
1	B	126	ASN
1	B	157	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 [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, 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%)	-0.10	20 (8%) 14 13	5, 10, 34, 59	0
1	B	244/252 (96%)	0.16	22 (9%) 12 12	5, 11, 49, 69	0
All	All	488/504 (96%)	0.03	42 (8%) 13 13	5, 10, 38, 69	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	THR	11.4
1	B	244	PRO	11.2
1	B	2	HIS	9.7
1	B	1	MET	8.5
1	B	203	ALA	8.5
1	A	2	HIS	8.2
1	B	214	LEU	8.2
1	B	207	PRO	6.4
1	A	208	THR	6.2
1	B	202	ARG	6.2
1	B	206	PHE	6.1
1	A	206	PHE	5.9
1	A	207	PRO	5.6
1	B	4	GLN	5.5
1	A	4	GLN	5.1
1	B	205	ALA	4.7
1	A	203	ALA	4.3
1	A	201	MET	4.1
1	A	245	GLY	3.8
1	B	199	THR	3.7
1	B	213[A]	LYS	3.5
1	A	1	MET	3.5
1	B	210	ASP	3.5
1	A	233[A]	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	205	ALA	3.3
1	A	200	ALA	3.0
1	B	215	LYS	3.0
1	B	196	GLY	3.0
1	B	211	PRO	2.9
1	B	200	ALA	2.9
1	B	209	GLU	2.9
1	B	204	SER	2.7
1	A	7	GLN	2.7
1	A	210	ASP	2.7
1	B	234	ARG	2.5
1	B	201	MET	2.2
1	A	202	ARG	2.2
1	A	244	PRO	2.2
1	A	45	ASN	2.2
1	A	213	LYS	2.1
1	A	211	PRO	2.1
1	A	209	GLU	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.