



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2018 – 01:33 PM EST

PDB ID : 5IUU  
Title : Crystal Structure of Indole-3-acetaldehyde Dehydrogenase in Apo form  
Authors : Lee, S.G.; McClerklin, S.; Kunkel, B.; Jez, J.M.  
Deposited on : 2016-03-18  
Resolution : 2.09 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

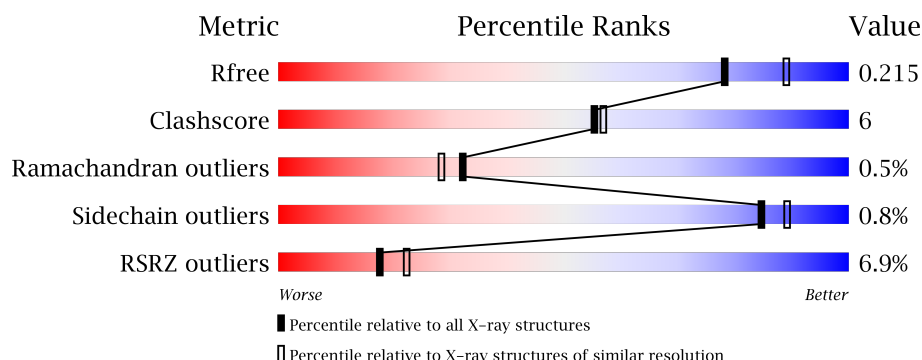
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	497	<div> <div>8%</div> <div>76%</div> <div>11%</div> <div>12%</div> </div>
1	B	497	<div> <div>4%</div> <div>77%</div> <div>8%</div> <div>15%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6787 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 Aldehyde dehydrogenase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3263	2070	561	620	12			
1	B	423	Total	C	N	O	S	0	0	0
			3162	2004	547	599	12			

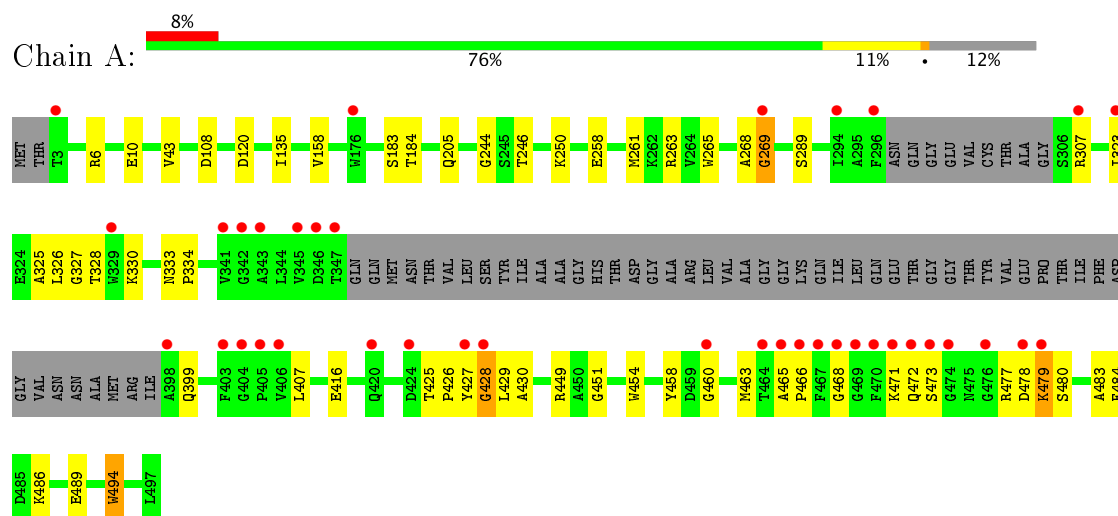
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	185	Total	O	0	0
			185	185		

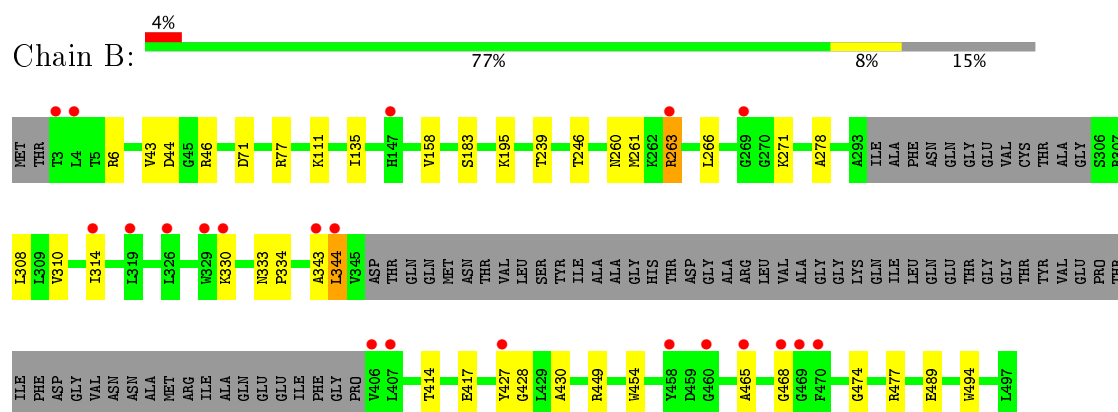
### 3 Residue-property plots [i](#)

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: Aldehyde dehydrogenase family protein



- Molecule 1: Aldehyde dehydrogenase family protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.89Å 109.07Å 143.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.45 – 2.09 40.44 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.45-2.09) 91.9 (40.44-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.197 , 0.222 0.189 , 0.215	Depositor DCC
$R_{free}$ test set	1843 reflections (2.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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, 0.333 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	0.41	0/3328	0.56	0/4525
1	B	0.40	0/3224	0.56	0/4383
All	All	0.40	0/6552	0.56	0/8908

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	3263	0	3268	56	0
1	B	3162	0	3177	28	0
2	A	177	0	0	6	1
2	B	185	0	0	2	1
All	All	6787	0	6445	76	1

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 6.

All (76) 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:258:GLU:OE2	2:A:501:HOH:O	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLU:OE2	2:A:503:HOH:O	1.91	0.86
1:A:427:TYR:HD2	1:A:471:LYS:HB3	1.43	0.83
1:A:454:TRP:NE1	1:A:460:GLY:O	2.12	0.81
1:A:425:THR:HG22	1:A:427:TYR:H	1.45	0.79
1:A:430:ALA:HB1	1:A:454:TRP:HZ3	1.53	0.73
1:A:463:MET:SD	1:A:479:LYS:HD2	2.30	0.72
1:A:468:GLY:HA3	1:A:477:ARG:HD3	1.73	0.71
1:A:449:ARG:NH1	2:A:507:HOH:O	2.24	0.69
1:A:399:GLN:NE2	2:A:508:HOH:O	2.25	0.68
1:A:325:ALA:O	1:A:328:THR:OG1	2.12	0.67
1:B:158:VAL:HG12	1:B:489:GLU:HG2	1.76	0.66
1:A:427:TYR:HB3	1:A:428:GLY:HA3	1.80	0.63
1:A:289:SER:HB2	1:A:458:TYR:CD2	2.34	0.62
1:A:265:TRP:CD2	1:A:486:LYS:HG2	2.37	0.60
1:A:307:ARG:NH2	1:A:425:THR:OG1	2.35	0.60
1:A:463:MET:HA	1:A:479:LYS:HE2	1.84	0.59
1:A:263:ARG:NE	1:A:489:GLU:OE1	2.32	0.59
1:B:71:ASP:O	1:B:77:ARG:NH2	2.36	0.58
1:A:6:ARG:NH1	1:A:333:ASN:HD22	2.01	0.58
1:B:343:ALA:O	1:B:344:LEU:HB2	2.07	0.53
1:A:451:GLY:HA3	1:A:468:GLY:O	2.09	0.53
1:A:465:ALA:HB2	1:B:494:TRP:CZ2	2.43	0.53
1:B:278:ALA:HA	1:B:314:ILE:HG12	1.89	0.53
1:A:425:THR:HG22	1:A:427:TYR:N	2.21	0.52
1:B:414:THR:OG1	1:B:417:GLU:HG3	2.09	0.52
1:A:269:GLY:O	1:A:429:LEU:HB2	2.10	0.51
1:B:43:VAL:HG22	1:B:334:PRO:HG2	1.92	0.51
1:A:108:ASP:O	2:A:505:HOH:O	2.20	0.51
1:A:454:TRP:HE1	1:A:460:GLY:C	2.10	0.51
1:A:184:THR:HG23	1:A:484:PHE:HD2	1.77	0.50
1:A:463:MET:SD	1:A:479:LYS:CD	3.00	0.50
1:A:135:ILE:HG12	1:A:183:SER:HB3	1.93	0.49
1:B:449:ARG:NH1	2:B:508:HOH:O	2.45	0.49
1:A:479:LYS:O	1:A:483:ALA:HB2	2.13	0.49
1:A:250:LYS:HG3	1:B:261:MET:HE2	1.95	0.48
1:A:268:ALA:O	1:A:473:SER:HA	2.13	0.48
1:B:430:ALA:HB1	1:B:454:TRP:CZ3	2.47	0.48
1:A:43:VAL:HG22	1:A:334:PRO:HG2	1.96	0.48
1:A:6:ARG:HD3	1:A:10:GLU:OE2	2.14	0.47
1:A:326:LEU:HD23	1:A:326:LEU:O	2.14	0.47
1:B:44:ASP:OD2	1:B:46:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ALA:O	1:A:479:LYS:HB2	2.15	0.47
1:A:471:LYS:HG3	1:A:472:GLN:H	1.79	0.47
1:B:468:GLY:HA3	1:B:477:ARG:HD3	1.96	0.46
1:A:246:THR:HG23	1:B:261:MET:CE	2.46	0.46
1:A:323:ILE:HD11	1:A:407:LEU:HD22	1.98	0.45
1:A:428:GLY:N	1:A:473:SER:OG	2.49	0.45
1:A:430:ALA:HB1	1:A:454:TRP:CZ3	2.41	0.45
1:A:425:THR:CG2	1:A:427:TYR:H	2.23	0.45
1:A:494:TRP:CZ2	1:B:465:ALA:HB2	2.51	0.45
1:A:416:GLU:CD	1:A:416:GLU:H	2.19	0.45
1:A:261:MET:CE	1:B:246:THR:HG23	2.47	0.45
1:A:471:LYS:NZ	2:A:510:HOH:O	2.40	0.45
1:A:158:VAL:HG12	1:A:489:GLU:HG2	2.00	0.44
1:B:195:LYS:O	2:B:501:HOH:O	2.21	0.44
1:A:466:PRO:HD3	1:A:480:SER:OG	2.19	0.43
1:B:271:LYS:HD3	1:B:427:TYR:HD1	1.82	0.43
1:A:427:TYR:CD2	1:A:471:LYS:HB3	2.35	0.43
1:A:244:GLY:O	1:A:268:ALA:HA	2.19	0.43
1:B:6:ARG:HE	1:B:333:ASN:HD22	1.67	0.42
1:A:466:PRO:HA	1:A:478:ASP:O	2.18	0.42
1:B:271:LYS:HD3	1:B:427:TYR:CD1	2.54	0.42
1:A:327:GLY:O	1:A:330:LYS:HE3	2.19	0.42
1:B:330:LYS:HG3	1:B:330:LYS:O	2.20	0.41
1:B:266:LEU:O	1:B:474:GLY:HA3	2.21	0.41
1:B:239:THR:OG1	1:B:263:ARG:NH1	2.49	0.41
1:A:426:PRO:O	1:A:427:TYR:HB2	2.20	0.41
1:A:465:ALA:HA	1:B:494:TRP:HZ2	1.84	0.41
1:A:427:TYR:CB	1:A:428:GLY:HA3	2.48	0.41
1:A:471:LYS:HE3	1:B:260:ASN:ND2	2.36	0.40
1:B:308:LEU:HG	1:B:310:VAL:CG2	2.50	0.40
1:A:265:TRP:HB3	1:A:486:LYS:HD3	2.03	0.40
1:B:135:ILE:HG12	1:B:183:SER:HB3	2.03	0.40
1:A:465:ALA:CB	1:B:494:TRP:CZ2	3.04	0.40
1:B:111:LYS:HB2	1:B:111:LYS:HE2	1.69	0.40

All (1) 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)
2:A:669:HOH:O	2:B:659:HOH:O[2_597]	2.17	0.03



## 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	430/497 (86%)	410 (95%)	18 (4%)	2 (0%)	32	28
1	B	417/497 (84%)	402 (96%)	13 (3%)	2 (0%)	32	28
All	All	847/994 (85%)	812 (96%)	31 (4%)	4 (0%)	32	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	GLY
1	A	428	GLY
1	B	344	LEU
1	B	428	GLY

### 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	334/380 (88%)	330 (99%)	4 (1%)	75	81
1	B	324/380 (85%)	323 (100%)	1 (0%)	94	96
All	All	658/760 (87%)	653 (99%)	5 (1%)	85	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASP
1	A	205	GLN

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Mol	Chain	Res	Type
1	A	479	LYS
1	A	494	TRP
1	B	263	ARG

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 [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	436/497 (87%)	0.40	38 (8%) 11 14	34, 45, 73, 87	0
1	B	423/497 (85%)	0.19	21 (4%) 30 36	32, 44, 65, 81	0
All	All	859/994 (86%)	0.30	59 (6%) 18 22	32, 45, 70, 87	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	PHE	7.1
1	A	471	LYS	6.1
1	A	473	SER	6.0
1	A	465	ALA	5.9
1	A	427	TYR	5.7
1	A	469	GLY	5.4
1	A	468	GLY	5.2
1	A	403	PHE	4.8
1	A	296	PHE	4.7
1	A	346	ASP	4.6
1	A	405	PRO	4.5
1	A	479	LYS	4.5
1	A	472	GLN	4.5
1	A	343	ALA	4.4
1	A	269	GLY	4.1
1	A	404	GLY	4.1
1	A	474	GLY	3.9
1	B	460	GLY	3.7
1	A	294	ILE	3.6
1	B	465	ALA	3.5
1	A	476	GLY	3.5
1	A	424	ASP	3.3
1	A	466	PRO	3.3
1	A	329	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	460	GLY	3.2
1	B	4	LEU	3.2
1	A	341	VAL	3.2
1	A	406	VAL	3.2
1	A	398	ALA	3.1
1	B	269	GLY	3.0
1	B	427	TYR	3.0
1	A	478	ASP	2.8
1	B	330	LYS	2.8
1	A	347	THR	2.8
1	B	406	VAL	2.7
1	A	464	THR	2.7
1	B	470	PHE	2.7
1	A	3	THR	2.7
1	B	344	LEU	2.6
1	A	467	PHE	2.6
1	B	458	TYR	2.6
1	A	428	GLY	2.5
1	B	468	GLY	2.5
1	B	314	ILE	2.5
1	B	343	ALA	2.3
1	B	147	HIS	2.3
1	A	307	ARG	2.3
1	A	420	GLN	2.3
1	A	342	GLY	2.3
1	B	329	TRP	2.3
1	A	176	TRP	2.3
1	A	345	VAL	2.2
1	B	326	LEU	2.1
1	A	323	ILE	2.1
1	B	407	LEU	2.1
1	B	3	THR	2.1
1	B	263	ARG	2.0
1	B	319	LEU	2.0
1	B	469	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.