



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:35 AM GMT

PDB ID : 3L6D  
Title : Crystal structure of putative oxidoreductase from *Pseudomonas putida* KT2440  
Authors : Malashkevich, V.N.; Patskovsky, Y.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYS-GXRC)  
Deposited on : 2009-12-23  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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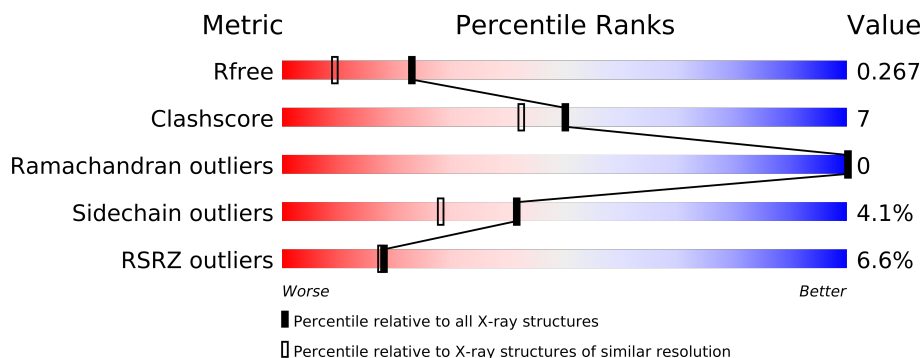
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	306	
1	B	306	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4780 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	Se	0	3	0
			2229	1412	402	407	2	6			
1	B	295	Total	C	N	O	S	Se	0	1	0
			2237	1413	403	412	2	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q88J51
A	2	SER	-	EXPRESSION TAG	UNP Q88J51
A	3	LEU	-	EXPRESSION TAG	UNP Q88J51
A	299	GLU	PRO	CONFLICT	UNP Q88J51
A	302	HIS	-	EXPRESSION TAG	UNP Q88J51
A	303	HIS	-	EXPRESSION TAG	UNP Q88J51
A	304	HIS	-	EXPRESSION TAG	UNP Q88J51
A	305	HIS	-	EXPRESSION TAG	UNP Q88J51
A	306	HIS	-	EXPRESSION TAG	UNP Q88J51
B	1	MSE	-	EXPRESSION TAG	UNP Q88J51
B	2	SER	-	EXPRESSION TAG	UNP Q88J51
B	3	LEU	-	EXPRESSION TAG	UNP Q88J51
B	299	GLU	PRO	CONFLICT	UNP Q88J51
B	302	HIS	-	EXPRESSION TAG	UNP Q88J51
B	303	HIS	-	EXPRESSION TAG	UNP Q88J51
B	304	HIS	-	EXPRESSION TAG	UNP Q88J51
B	305	HIS	-	EXPRESSION TAG	UNP Q88J51
B	306	HIS	-	EXPRESSION TAG	UNP Q88J51

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		

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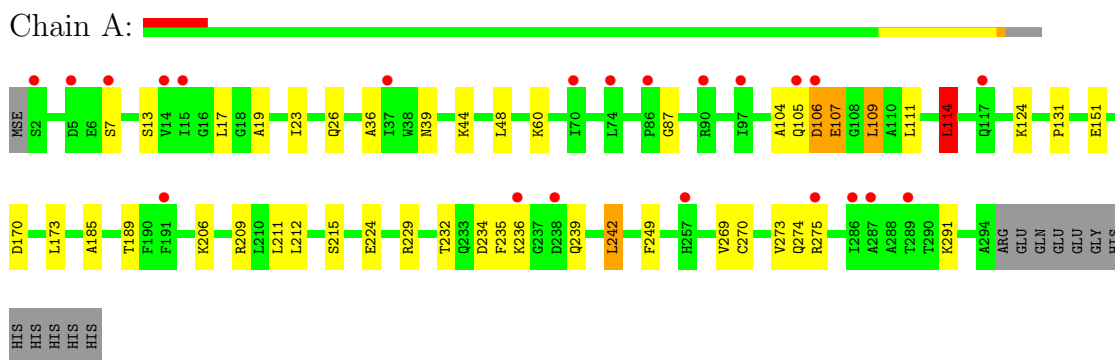
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	175	Total	O	0	0
			175	175		

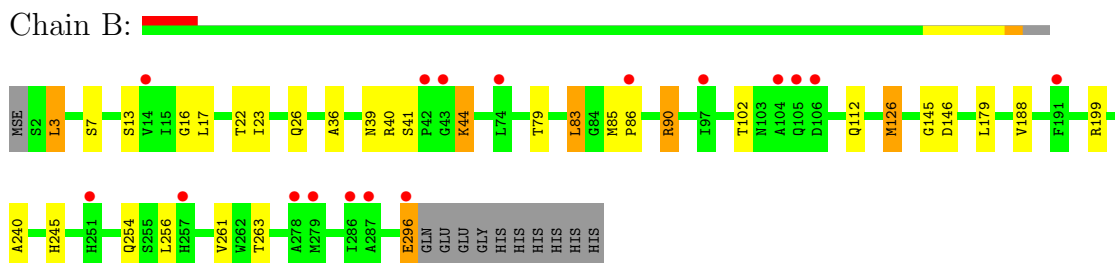
### 3 Residue-property plots

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: Putative oxidoreductase



#### • Molecule 1: Putative oxidoreductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.34Å 37.65Å 104.25Å 90.00° 93.35° 90.00°	Depositor
Resolution (Å)	19.94 – 1.90 19.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-1.90) 98.5 (19.92-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.208 , 0.260 0.215 , 0.267	Depositor DCC
$R_{free}$ test set	2610 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 51537 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.75	0/2280	0.73	4/3085 (0.1%)
1	B	0.79	0/2278	0.72	1/3081 (0.0%)
All	All	0.77	0/4558	0.73	5/6166 (0.1%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	114	LEU	CA-CB-CG	6.73	130.79	115.30
1	A	242	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	3	LEU	CA-CB-CG	6.53	130.33	115.30
1	A	170	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	209	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	THR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2229	0	2199	39	0
1	B	2237	0	2195	30	1
2	A	139	0	0	5	0
2	B	175	0	0	1	0
All	All	4780	0	4394	66	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (66) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:104:ALA:O	1:A:107:GLU:HG3	1.58	1.02
1:A:17:LEU:O	1:A:44:LYS:HG2	1.72	0.88
1:A:19:ALA:O	1:A:23:ILE:HG12	1.74	0.86
1:A:270:CYS:O	1:A:274:GLN:HG2	1.75	0.86
1:A:60:LYS:HE2	1:A:87:GLY:HA3	1.66	0.78
1:A:124:LYS:HE2	1:A:173:LEU:HD21	1.69	0.75
1:B:17:LEU:HG	1:B:39:ASN:HB2	1.69	0.74
1:A:212:LEU:HD12	2:A:347:HOH:O	1.91	0.70
1:B:39:ASN:HD22	1:B:41:SER:N	1.90	0.70
1:A:17:LEU:HD12	1:A:39:ASN:HB2	1.79	0.64
1:A:151:GLU:HG3	2:A:364:HOH:O	1.98	0.63
1:B:39:ASN:ND2	1:B:40:ARG:H	2.00	0.59
1:A:109:LEU:HD12	1:A:109:LEU:N	2.19	0.57
1:A:206:LYS:HE2	2:A:441:HOH:O	2.03	0.57
1:B:23:ILE:HD12	1:B:26:GLN:HE21	1.70	0.57
1:A:109:LEU:CD1	1:A:109:LEU:N	2.68	0.57
1:B:23:ILE:HD12	1:B:26:GLN:NE2	2.20	0.56
1:A:109:LEU:CD1	1:A:109:LEU:H	2.18	0.56
1:A:104:ALA:O	1:A:107:GLU:CG	2.46	0.55
1:A:212:LEU:CD1	2:A:347:HOH:O	2.54	0.55
1:B:256:LEU:HD13	1:B:263:THR:HG21	1.88	0.54
1:A:106:ASP:H	1:A:109:LEU:HD13	1.73	0.54
1:B:261:VAL:HG23	1:B:263:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:39:ASN:HD22	1:B:41:SER:H	1.55	0.53
1:A:211[A]:LEU:HD11	1:B:179:LEU:HA	1.92	0.52
1:A:106:ASP:HA	1:A:109:LEU:HD13	1.92	0.52
1:A:224:GLU:HG2	2:A:382:HOH:O	2.10	0.51
1:A:106:ASP:CA	1:A:109:LEU:HD13	2.40	0.51
1:A:60:LYS:HE2	1:A:87:GLY:CA	2.41	0.49
1:A:105:GLN:O	1:A:106:ASP:OD1	2.29	0.49
1:A:23:ILE:HG13	1:A:131:PRO:HB3	1.95	0.47
1:B:85:MSE:HB3	1:B:86:PRO:HD2	1.97	0.47
1:A:106:ASP:HA	1:A:109:LEU:HD22	1.96	0.47
1:A:17:LEU:O	1:A:44:LYS:CG	2.54	0.47
1:B:16:GLY:O	1:B:17:LEU:HD23	2.16	0.46
1:B:39:ASN:CG	1:B:40:ARG:H	2.19	0.45
1:B:240:ALA:HB1	1:B:245:HIS:CE1	2.51	0.45
1:A:26:GLN:HG3	1:A:48:LEU:HD21	1.97	0.45
1:B:39:ASN:ND2	1:B:40:ARG:N	2.65	0.45
1:A:114:LEU:HD12	1:A:114:LEU:C	2.36	0.45
1:A:232:THR:HG23	1:A:234:ASP:HB3	1.98	0.45
1:B:16:GLY:HA2	1:B:39:ASN:OD1	2.17	0.45
1:B:112:GLN:NE2	1:B:145:GLY:HA2	2.32	0.44
1:B:17:LEU:CD1	1:B:39:ASN:HB2	2.48	0.44
1:B:17:LEU:CG	1:B:39:ASN:HB2	2.44	0.44
1:A:269:VAL:HG13	1:B:188:VAL:HG21	1.99	0.44
1:A:215:SER:HB3	1:B:179:LEU:HD11	2.00	0.44
1:B:126[B]:MSE:HB2	1:B:126[B]:MSE:HE3	1.81	0.44
1:B:79:THR:O	1:B:83:LEU:CD2	2.67	0.43
1:A:232:THR:HG23	1:A:234:ASP:CB	2.49	0.43
1:B:79:THR:O	1:B:83:LEU:HD22	2.19	0.43
1:B:13:SER:HA	1:B:36:ALA:O	2.19	0.42
1:B:146:ASP:HB2	2:B:365:HOH:O	2.18	0.42
1:A:13:SER:HA	1:A:36:ALA:O	2.19	0.42
1:B:240:ALA:HB1	1:B:245:HIS:HE1	1.82	0.42
1:A:105:GLN:O	1:A:106:ASP:CB	2.68	0.42
1:A:106:ASP:N	1:A:109:LEU:HD13	2.34	0.42
1:A:185:ALA:O	1:A:189:THR:HG23	2.19	0.42
1:A:235:PHE:CZ	1:A:291:LYS:HD2	2.55	0.42
1:B:199:ARG:HD2	1:B:261:VAL:HG12	2.01	0.41
1:B:22:THR:OG1	1:B:44:LYS:HG2	2.20	0.41
1:A:249:PHE:CE2	1:A:273:VAL:HG21	2.56	0.41
1:B:16:GLY:C	1:B:17:LEU:HD23	2.41	0.40
1:A:229:ARG:HA	1:A:232:THR:HG22	2.03	0.40
1:A:232:THR:CG2	1:A:234:ASP:HB3	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:GLU:H	1:B:296:GLU:HG3	1.38	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	Distance(Å)	Clash(Å)
1:B:90:ARG:NH2	1:B:296:GLU:OE1[2_555]	2.18	0.02

## 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	294/306 (96%)	287 (98%)	7 (2%)	0	100	100
1	B	294/306 (96%)	286 (97%)	8 (3%)	0	100	100
All	All	588/612 (96%)	573 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	222/224 (99%)	212 (96%)	10 (4%)	38	24
1	B	222/224 (99%)	213 (96%)	9 (4%)	41	28
All	All	444/448 (99%)	425 (96%)	19 (4%)	41	26

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	106	ASP
1	A	107	GLU
1	A	109	LEU
1	A	111	LEU
1	A	114	LEU
1	A	236	LYS
1	A	239	GLN
1	A	242	LEU
1	A	275	ARG
1	B	3	LEU
1	B	7	SER
1	B	44	LYS
1	B	83	LEU
1	B	90	ARG
1	B	126[A]	MSE
1	B	126[B]	MSE
1	B	254	GLN
1	B	296	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	80	HIS
1	A	140	HIS
1	B	26	GLN
1	B	39	ASN
1	B	112	GLN
1	B	116	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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 ⓘ

### 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	293/306 (95%)	0.36	22 (7%) 14 14	19, 30, 48, 66	0
1	B	295/306 (96%)	0.37	17 (5%) 22 22	16, 27, 45, 68	0
All	All	588/612 (96%)	0.36	39 (6%) 18 17	16, 29, 48, 68	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ASP	5.3
1	B	105	GLN	4.6
1	B	257	HIS	4.5
1	B	296	GLU	4.1
1	B	43	GLY	4.0
1	A	74	LEU	3.9
1	B	74	LEU	3.8
1	B	104	ALA	3.5
1	A	286	ILE	3.4
1	B	191	PHE	3.1
1	A	15	ILE	2.9
1	A	287	ALA	2.8
1	A	70	ILE	2.7
1	A	105	GLN	2.7
1	A	7	SER	2.7
1	A	106	ASP	2.6
1	B	86	PRO	2.6
1	B	42	PRO	2.5
1	B	278	ALA	2.5
1	B	286	ILE	2.5
1	A	90	ARG	2.5
1	A	191	PHE	2.4
1	A	236	LYS	2.4
1	A	238	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	289	THR	2.4
1	A	86	PRO	2.3
1	A	37	ILE	2.2
1	A	97	ILE	2.2
1	B	106	ASP	2.2
1	B	287	ALA	2.2
1	B	251	HIS	2.2
1	A	2	SER	2.2
1	B	97	ILE	2.2
1	A	117	GLN	2.2
1	B	279	MSE	2.2
1	A	275	ARG	2.1
1	A	14	VAL	2.1
1	B	14	VAL	2.1
1	A	257	HIS	2.1

## 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 ⓘ

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.