



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 PM GMT

PDB ID : 4LN9  
Title : Crystal structure of the dehydratase domain from the terminal module of the rifamycin polyketide synthase  
Authors : Gay, D.C.; You, Y.-O.; Cane, D.; Keatinge-Clay, A.T.  
Deposited on : 2013-07-11  
Resolution : 1.82 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

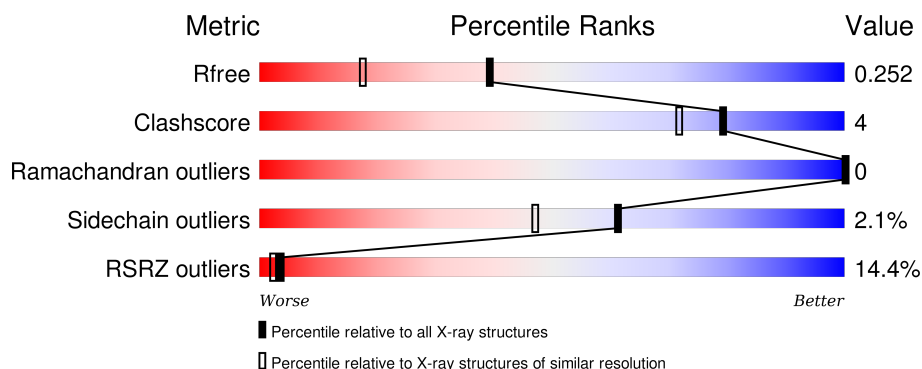
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

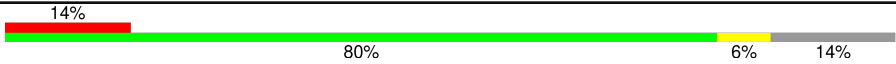

The reported resolution of this entry is 1.82 Å.

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	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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	325	
1	B	325	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4444 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 Rifamycin polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2086	1314	380	390	2			
1	B	276	Total	C	N	O	S	0	0	0
			2048	1291	372	383	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O54593
A	-18	GLY	-	EXPRESSION TAG	UNP O54593
A	-17	SER	-	EXPRESSION TAG	UNP O54593
A	-16	SER	-	EXPRESSION TAG	UNP O54593
A	-15	HIS	-	EXPRESSION TAG	UNP O54593
A	-14	HIS	-	EXPRESSION TAG	UNP O54593
A	-13	HIS	-	EXPRESSION TAG	UNP O54593
A	-12	HIS	-	EXPRESSION TAG	UNP O54593
A	-11	HIS	-	EXPRESSION TAG	UNP O54593
A	-10	HIS	-	EXPRESSION TAG	UNP O54593
A	-9	SER	-	EXPRESSION TAG	UNP O54593
A	-8	SER	-	EXPRESSION TAG	UNP O54593
A	-7	GLY	-	EXPRESSION TAG	UNP O54593
A	-6	LEU	-	EXPRESSION TAG	UNP O54593
A	-5	VAL	-	EXPRESSION TAG	UNP O54593
A	-4	PRO	-	EXPRESSION TAG	UNP O54593
A	-3	ARG	-	EXPRESSION TAG	UNP O54593
A	-2	GLY	-	EXPRESSION TAG	UNP O54593
A	-1	SER	-	EXPRESSION TAG	UNP O54593
A	0	HIS	-	EXPRESSION TAG	UNP O54593
A	1	MET	-	EXPRESSION TAG	UNP O54593
B	-19	MET	-	EXPRESSION TAG	UNP O54593
B	-18	GLY	-	EXPRESSION TAG	UNP O54593
B	-17	SER	-	EXPRESSION TAG	UNP O54593
B	-16	SER	-	EXPRESSION TAG	UNP O54593

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP O54593
B	-14	HIS	-	EXPRESSION TAG	UNP O54593
B	-13	HIS	-	EXPRESSION TAG	UNP O54593
B	-12	HIS	-	EXPRESSION TAG	UNP O54593
B	-11	HIS	-	EXPRESSION TAG	UNP O54593
B	-10	HIS	-	EXPRESSION TAG	UNP O54593
B	-9	SER	-	EXPRESSION TAG	UNP O54593
B	-8	SER	-	EXPRESSION TAG	UNP O54593
B	-7	GLY	-	EXPRESSION TAG	UNP O54593
B	-6	LEU	-	EXPRESSION TAG	UNP O54593
B	-5	VAL	-	EXPRESSION TAG	UNP O54593
B	-4	PRO	-	EXPRESSION TAG	UNP O54593
B	-3	ARG	-	EXPRESSION TAG	UNP O54593
B	-2	GLY	-	EXPRESSION TAG	UNP O54593
B	-1	SER	-	EXPRESSION TAG	UNP O54593
B	0	HIS	-	EXPRESSION TAG	UNP O54593
B	1	MET	-	EXPRESSION TAG	UNP O54593

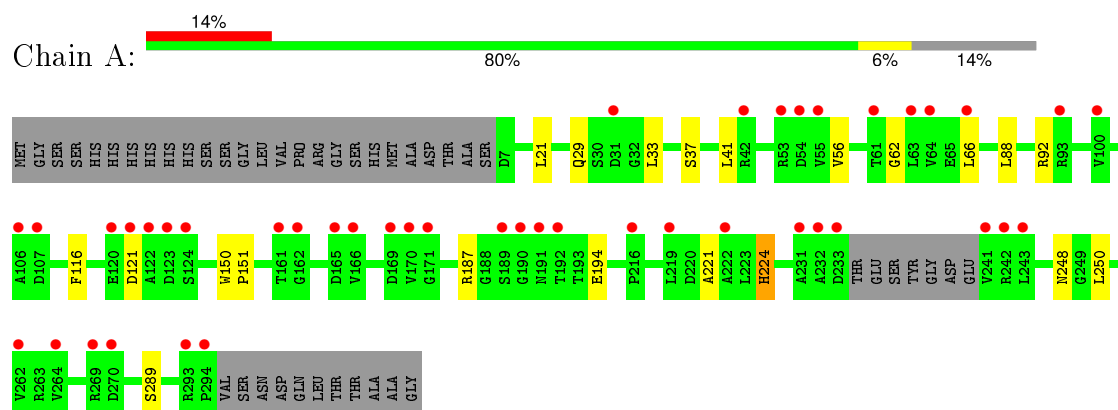
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	136	Total O 136 136	0	0
2	B	174	Total O 174 174	0	0

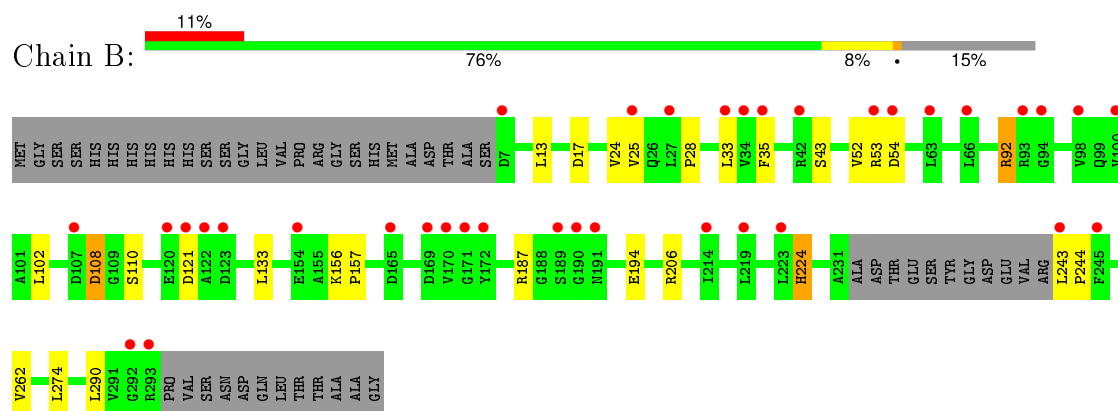
### 3 Residue-property plots [i](#)

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: Rifamycin polyketide synthase



#### • Molecule 1: Rifamycin polyketide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.18 Å 77.18 Å 97.92 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.50 – 1.82 29.33 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.50-1.82) 99.2 (29.33-1.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.82 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.211 , 0.254 0.210 , 0.252	Depositor DCC
$R_{free}$ test set	2960 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 54.1	EDS
Estimated twinning fraction	0.008 for -h,-k,l 0.035 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 58034 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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	0.41	0/2132	0.44	0/2916
1	B	0.42	0/2093	0.45	0/2862
All	All	0.41	0/4225	0.44	0/5778

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	108	ASP	Mainchain
1	B	121	ASP	Peptide

### 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	2086	0	2072	13	0
1	B	2048	0	2034	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	136	0	0	1	0
2	B	174	0	0	4	0
All	All	4444	0	4106	29	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 4.

All (29) 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:54:ASP:O	1:B:92:ARG:NH2	2.22	0.71
1:A:41:LEU:HD12	1:A:92:ARG:HD3	1.76	0.68
1:B:108:ASP:HB3	1:B:110:SER:H	1.64	0.63
1:B:102:LEU:HD11	1:B:133:LEU:HD12	1.85	0.57
1:A:187:ARG:HD2	1:A:194:GLU:OE1	2.07	0.54
1:B:13:LEU:HD23	1:B:25:VAL:HB	1.91	0.52
1:A:33:LEU:HD12	1:A:33:LEU:C	2.29	0.52
1:A:62:GLY:O	1:A:66:LEU:HG	2.10	0.52
1:B:52:VAL:O	1:B:53:ARG:HG3	2.10	0.52
1:B:244:PRO:HB2	1:B:290:LEU:HD11	1.91	0.52
1:A:92:ARG:NH2	2:A:478:HOH:O	2.43	0.51
1:A:221:ALA:HA	1:A:224:HIS:CE1	2.46	0.51
1:A:41:LEU:CD1	1:A:92:ARG:HD3	2.41	0.50
1:B:206:ARG:NH2	2:B:495:HOH:O	2.42	0.49
1:A:248:ASN:HB2	1:A:289:SER:HB3	1.94	0.48
1:A:21:LEU:HA	1:A:37:SER:HB2	1.94	0.48
1:B:262:VAL:HG13	1:B:274:LEU:CD1	2.44	0.48
1:B:33:LEU:HD13	1:B:35:PHE:CE1	2.50	0.47
1:B:243:LEU:N	2:B:520:HOH:O	2.48	0.46
1:B:187:ARG:HD2	1:B:194:GLU:OE1	2.16	0.46
1:B:156:LYS:HA	1:B:157:PRO:HD3	1.87	0.44
1:A:41:LEU:HD21	1:A:56:VAL:HG11	2.00	0.42
1:B:262:VAL:HG13	1:B:274:LEU:HD12	2.02	0.42
1:A:29:GLN:HG2	2:B:478:HOH:O	2.20	0.42
1:A:116:PHE:CD2	1:B:28:PRO:HG2	2.55	0.42
1:A:150:TRP:HA	1:A:151:PRO:C	2.40	0.41
1:B:224:HIS:C	1:B:224:HIS:CD2	2.93	0.41
1:B:244:PRO:HA	2:B:446:HOH:O	2.21	0.41
1:B:92:ARG:HA	1:B:92:ARG:HD3	1.65	0.40

There are no symmetry-related clashes.



## 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	277/325 (85%)	271 (98%)	6 (2%)	0	100	100
1	B	272/325 (84%)	263 (97%)	9 (3%)	0	100	100
All	All	549/650 (84%)	534 (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	213/248 (86%)	209 (98%)	4 (2%)	65	52
1	B	209/248 (84%)	204 (98%)	5 (2%)	57	40
All	All	422/496 (85%)	413 (98%)	9 (2%)	61	47

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

Mol	Chain	Res	Type
1	A	88	LEU
1	A	121	ASP
1	A	224	HIS
1	A	250	LEU
1	B	17	ASP
1	B	24	VAL
1	B	43	SER
1	B	92	ARG

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Mol	Chain	Res	Type
1	B	224	HIS

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	281/325 (86%)	0.77	44 (15%) <b>3</b> <b>2</b>	22, 37, 66, 87	0
1	B	276/325 (84%)	0.63	36 (13%) <b>5</b> <b>3</b>	23, 35, 61, 81	0
All	All	557/650 (85%)	0.70	80 (14%) <b>3</b> <b>2</b>	22, 36, 65, 87	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	6.5
1	B	243	LEU	6.2
1	A	294	PRO	6.0
1	A	191	ASN	5.5
1	A	190	GLY	5.4
1	B	121	ASP	5.2
1	A	189	SER	5.1
1	A	169	ASP	5.0
1	A	269	ARG	4.9
1	A	123	ASP	4.4
1	B	123	ASP	4.4
1	A	121	ASP	4.3
1	A	293	ARG	4.0
1	B	191	ASN	4.0
1	B	53	ARG	3.9
1	A	54	ASP	3.9
1	B	293	ARG	3.9
1	B	171	GLY	3.8
1	A	171	GLY	3.8
1	B	100	VAL	3.7
1	B	190	GLY	3.7
1	A	170	VAL	3.6
1	A	93	ARG	3.6
1	B	66	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	98	VAL	3.5
1	A	232	ALA	3.5
1	B	169	ASP	3.4
1	B	107	ASP	3.4
1	A	231	ALA	3.4
1	A	120	GLU	3.3
1	A	233	ASP	3.3
1	A	106	ALA	3.3
1	A	219	LEU	3.2
1	B	154	GLU	3.2
1	B	189	SER	3.2
1	B	42	ARG	3.2
1	B	219	LEU	3.1
1	A	192	THR	3.1
1	A	243	LEU	3.1
1	A	165	ASP	3.1
1	A	63	LEU	3.0
1	B	93	ARG	3.0
1	A	53	ARG	2.8
1	B	170	VAL	2.8
1	B	35	PHE	2.7
1	B	25	VAL	2.7
1	B	7	ASP	2.6
1	B	122	ALA	2.6
1	B	292	GLY	2.6
1	A	242	ARG	2.5
1	B	54	ASP	2.5
1	A	161	THR	2.5
1	A	42	ARG	2.5
1	B	223	LEU	2.5
1	B	34	VAL	2.4
1	B	63	LEU	2.4
1	A	262	VAL	2.4
1	B	94	GLY	2.4
1	A	31	ASP	2.4
1	A	107	ASP	2.4
1	B	165	ASP	2.3
1	A	124	SER	2.3
1	A	64	VAL	2.3
1	A	222	ALA	2.3
1	B	214	ILE	2.3
1	A	270	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	27	LEU	2.2
1	A	166	VAL	2.2
1	B	120	GLU	2.2
1	B	245	PHE	2.2
1	A	122	ALA	2.2
1	A	66	LEU	2.2
1	A	55	VAL	2.2
1	A	162	GLY	2.2
1	A	100	VAL	2.2
1	B	172	TYR	2.2
1	A	61	THR	2.1
1	B	33	LEU	2.1
1	A	216	PRO	2.1
1	A	264	VAL	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 ⓘ

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.