



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:45 AM GMT

PDB ID : 2W2F  
Title : CRYSTAL STRUCTURE OF SINGLE POINT MUTANT ARG48GLN OF P-COUMARIC ACID DECARBOXYLASE FROM LACTOBACILLUS PLANTARUM STRUCTURAL INSIGHTS INTO THE ACTIVE SITE AND DECARBOXYLATION CATALYTIC MECHANISM  
Authors : Rodriguez, H.; Angulo, I.; De Las Rivas, B.; Campillo, N.; Paez, J.A.; Munoz, R.; Mancheno, J.M.  
Deposited on : 2008-10-29  
Resolution : 1.73 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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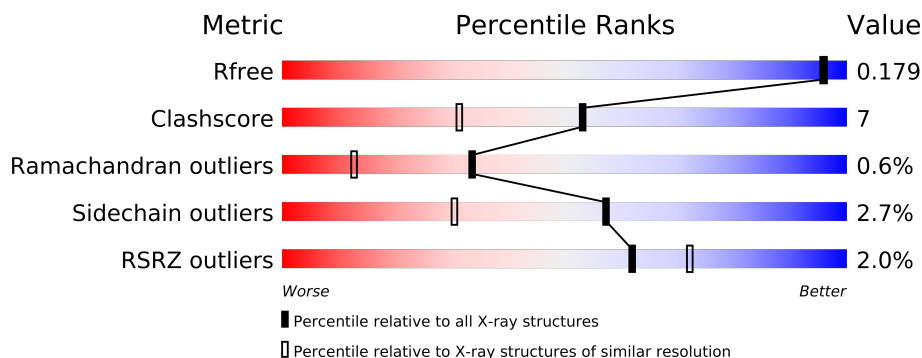
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **FAILED**  
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 1.73 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	1657 (1.76-1.72)
Clashscore	79885	1881 (1.76-1.72)
Ramachandran outliers	78287	1859 (1.76-1.72)
Sidechain outliers	78261	1859 (1.76-1.72)
RSRZ outliers	66119	1658 (1.76-1.72)

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	194	
1	B	194	
1	C	194	
1	D	194	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6326 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 P-COUMARIC ACID DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1457	936	234	281	6			
1	B	175	Total	C	N	O	S	0	0	0
			1457	936	234	281	6			
1	C	175	Total	C	N	O	S	0	0	0
			1457	936	234	281	6			
1	D	175	Total	C	N	O	S	0	0	0
			1457	936	234	281	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLN	ARG	ENGINEERED MUTATION	UNP Q88RY7
B	48	GLN	ARG	ENGINEERED MUTATION	UNP Q88RY7
C	48	GLN	ARG	ENGINEERED MUTATION	UNP Q88RY7
D	48	GLN	ARG	ENGINEERED MUTATION	UNP Q88RY7

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ba	0	0
			1	1		
2	D	1	Total	Ba	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	126	Total	O	0	0
			126	126		

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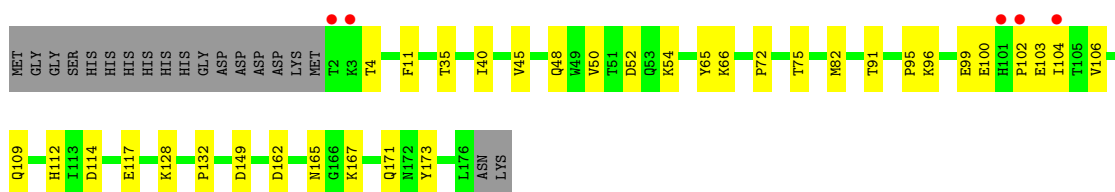
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	117	Total 117	O 117	0	0
3	D	138	Total 138	O 138	0	0

### 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.

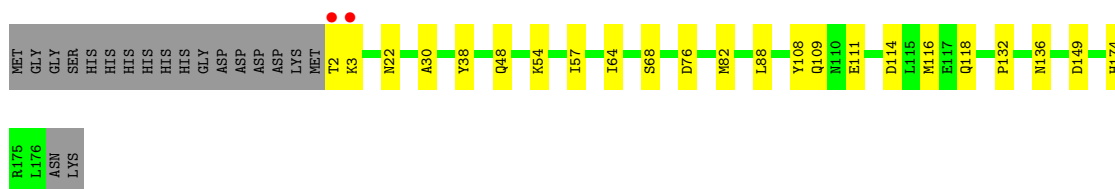
- Molecule 1: P-COUMARIC ACID DECARBOXYLASE

Chain A:



- Molecule 1: P-COUMARIC ACID DECARBOXYLASE

Chain B:



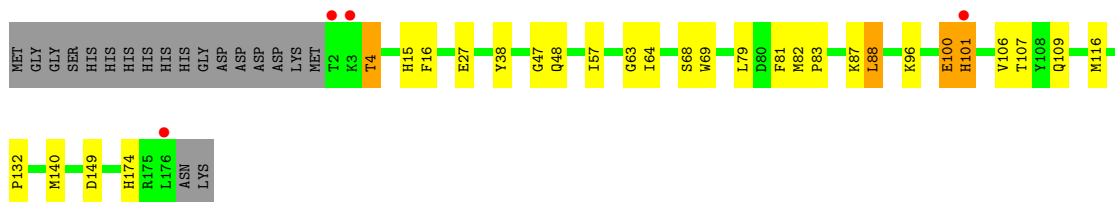
- Molecule 1: P-COUMARIC ACID DECARBOXYLASE

Chain C:



- Molecule 1: P-COUMARIC ACID DECARBOXYLASE

Chain D:



## 4 Data and refinement statistics

Xtrriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.25Å 94.92Å 106.72Å 90.00° 100.51° 90.00°	Depositor
Resolution (Å)	35.76 – 1.73 35.75 – 1.73	Depositor EDS
% Data completeness (in resolution range)	69.7 (35.76-1.73) 69.4 (35.75-1.73)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.226 , 0.273 0.164 , 0.179	Depositor DCC
$R_{free}$ test set	2830 reflections (5.33%)	DCC
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 24.7	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
BA

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	0.49	0/1502	0.61	0/2043
1	B	0.51	0/1502	0.60	1/2043 (0.0%)
1	C	0.51	0/1502	0.64	0/2043
1	D	0.53	0/1502	0.62	1/2043 (0.0%)
All	All	0.51	0/6008	0.62	2/8172 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	LEU	CA-CB-CG	5.34	127.59	115.30
1	D	88	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1457	0	1358	25	0
1	B	1457	0	1358	18	0
1	C	1457	0	1358	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1457	0	1358	25	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	115	0	0	9	0
3	B	126	0	0	12	0
3	C	117	0	0	7	0
3	D	138	0	0	16	0
All	All	6326	0	5432	79	0

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:107:THR:HB	3:D:2080:HOH:O	1.34	1.21
1:C:15:HIS:HB3	3:C:2116:HOH:O	1.38	1.19
1:A:114:ASP:HB3	3:A:2072:HOH:O	1.55	1.04
1:B:64:ILE:HD12	1:B:82:MET:HG2	1.54	0.89
1:B:111:GLU:HG2	3:B:2074:HOH:O	1.72	0.88
1:D:69:TRP:HZ3	3:D:2031:HOH:O	1.58	0.86
1:A:117:GLU:HG3	3:A:2070:HOH:O	1.76	0.85
1:B:114:ASP:O	1:B:118:GLN:HG3	1.80	0.82
1:D:100:GLU:HG2	3:D:2075:HOH:O	1.80	0.82
1:A:165:ASN:HB2	1:A:167:LYS:HE2	1.65	0.78
1:B:38:TYR:OH	1:B:48:GLN:NE2	2.16	0.78
1:D:15:HIS:CD2	3:D:2017:HOH:O	2.38	0.77
1:C:101:HIS:HE1	3:C:2058:HOH:O	1.68	0.75
1:D:4:THR:HG22	3:D:2006:HOH:O	1.88	0.73
1:A:82:MET:HG3	3:A:2049:HOH:O	1.88	0.73
1:D:38:TYR:OH	1:D:48:GLN:NE2	2.21	0.73
1:B:174:HIS:HE1	3:B:2122:HOH:O	1.71	0.72
1:A:162:ASP:HA	1:A:167:LYS:HE3	1.75	0.67
1:D:101:HIS:HB3	3:D:2076:HOH:O	1.95	0.66
1:A:82:MET:CE	3:A:2049:HOH:O	2.45	0.65
1:D:64:ILE:HD12	1:D:82:MET:HG2	1.79	0.64
3:A:2072:HOH:O	1:C:174:HIS:HE1	1.79	0.64
1:C:64:ILE:HD12	1:C:82:MET:HG3	1.80	0.64
1:D:27:GLU:CG	3:D:2017:HOH:O	2.46	0.62
1:A:114:ASP:HB3	3:A:2075:HOH:O	2.00	0.60
1:D:27:GLU:HG3	3:D:2017:HOH:O	2.02	0.59
1:D:16:PHE:CD2	1:D:140:MET:HG2	2.40	0.57
1:D:27:GLU:HG2	3:D:2017:HOH:O	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:57:ILE:HD13	3:D:2032:HOH:O	2.06	0.55
1:B:57:ILE:HD13	3:B:2028:HOH:O	2.07	0.54
1:B:38:TYR:HE1	3:B:2045:HOH:O	1.91	0.54
1:B:3:LYS:HD3	3:B:2003:HOH:O	2.08	0.53
1:B:174:HIS:CE1	3:B:2122:HOH:O	2.55	0.53
1:D:79:LEU:HD12	3:D:2031:HOH:O	2.09	0.53
1:D:96:LYS:NZ	1:D:100:GLU:OE1	2.39	0.52
1:C:174:HIS:HD2	3:C:2112:HOH:O	1.91	0.52
1:A:112:HIS:ND1	1:C:148:GLU:OE2	2.41	0.52
1:C:107:THR:HG21	3:C:2062:HOH:O	2.10	0.52
1:C:42:GLY:HA3	3:C:2015:HOH:O	2.09	0.51
1:B:109:GLN:OE1	1:B:116:MET:SD	2.69	0.51
1:A:50:VAL:HG22	1:A:109:GLN:HB3	1.94	0.50
1:B:136:ASN:ND2	3:B:2094:HOH:O	2.44	0.50
1:B:54:LYS:HD3	3:B:2031:HOH:O	2.13	0.49
1:D:106:VAL:O	1:D:106:VAL:HG12	2.12	0.48
1:A:40:ILE:HD12	1:A:48:GLN:HB3	1.95	0.48
1:C:91:THR:HG21	1:D:68:SER:HB3	1.95	0.48
1:A:72:PRO:HB3	3:A:2070:HOH:O	2.13	0.48
1:A:75:THR:HA	1:A:95:PRO:HD3	1.95	0.48
1:B:30:ALA:HB1	3:B:2028:HOH:O	2.15	0.47
1:D:109:GLN:HG2	1:D:116:MET:HG3	1.96	0.47
1:A:102:PRO:O	1:A:106:VAL:HG23	2.15	0.47
1:D:69:TRP:CZ3	3:D:2031:HOH:O	2.45	0.47
1:D:174:HIS:HE1	3:D:2135:HOH:O	1.97	0.46
1:A:171:GLN:HG2	1:A:171:GLN:O	2.15	0.46
1:D:15:HIS:HD2	3:D:2017:HOH:O	1.87	0.45
1:C:97:TRP:HA	1:C:100:GLU:HB2	1.99	0.45
1:A:66:LYS:HE3	3:B:2064:HOH:O	2.17	0.45
1:A:40:ILE:HD13	1:A:45:VAL:HG23	1.99	0.44
1:B:109:GLN:NE2	3:B:2072:HOH:O	2.50	0.44
1:A:82:MET:CG	3:A:2049:HOH:O	2.55	0.44
1:D:81:PHE:CE2	1:D:88:LEU:HD12	2.52	0.44
1:A:35:THR:CG2	1:A:52:ASP:HA	2.47	0.44
1:A:91:THR:HG21	1:B:68:SER:HB3	1.99	0.44
1:C:114:ASP:HB3	3:C:2071:HOH:O	2.18	0.44
1:C:122:LYS:HD3	1:C:123:TYR:CZ	2.52	0.44
1:D:63:GLY:O	1:D:83:PRO:HD2	2.19	0.43
1:A:54:LYS:HD3	1:A:54:LYS:HA	1.82	0.42
1:D:47:GLY:HA3	1:D:106:VAL:HG13	2.00	0.42
1:C:114:ASP:CG	3:C:2071:HOH:O	2.58	0.42
1:D:100:GLU:HG2	3:D:2074:HOH:O	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:44:MET:O	1:C:102:PRO:HB2	2.21	0.41
1:A:128:LYS:NZ	1:B:76:ASP:OD2	2.47	0.41
1:A:99:GLU:O	1:A:99:GLU:HG2	2.19	0.41
1:B:64:ILE:HD11	3:B:2066:HOH:O	2.19	0.41
1:A:103:GLU:HG2	1:A:104:ILE:N	2.36	0.41
1:A:96:LYS:HA	3:A:2053:HOH:O	2.21	0.40
1:A:11:PHE:HB2	1:A:65:TYR:CZ	2.56	0.40
1:B:108:TYR:HD2	1:B:111:GLU:OE1	2.04	0.40
1:C:66:LYS:HE3	3:D:2066:HOH:O	2.21	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	173/194 (89%)	167 (96%)	5 (3%)	1 (1%)	33	13
1	B	173/194 (89%)	166 (96%)	6 (4%)	1 (1%)	33	13
1	C	173/194 (89%)	164 (95%)	8 (5%)	1 (1%)	33	13
1	D	173/194 (89%)	168 (97%)	4 (2%)	1 (1%)	33	13
All	All	692/776 (89%)	665 (96%)	23 (3%)	4 (1%)	33	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	PRO
1	D	132	PRO
1	C	132	PRO
1	A	132	PRO

### 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	156/172 (91%)	152 (97%)	4 (3%)	59	32
1	B	156/172 (91%)	153 (98%)	3 (2%)	69	47
1	C	156/172 (91%)	151 (97%)	5 (3%)	51	22
1	D	156/172 (91%)	151 (97%)	5 (3%)	51	22
All	All	624/688 (91%)	607 (97%)	17 (3%)	57	30

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	100	GLU
1	A	149	ASP
1	A	173	TYR
1	B	2	THR
1	B	22	ASN
1	B	149	ASP
1	C	96	LYS
1	C	100	GLU
1	C	114	ASP
1	C	149	ASP
1	C	173	TYR
1	D	4	THR
1	D	87	LYS
1	D	100	GLU
1	D	101	HIS
1	D	149	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	174	HIS
1	B	22	ASN
1	B	48	GLN

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Mol	Chain	Res	Type
1	B	109	GLN
1	B	136	ASN
1	B	174	HIS
1	C	101	HIS
1	C	174	HIS
1	D	48	GLN
1	D	109	GLN
1	D	174	HIS

### 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

### 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	175/194 (90%)	-0.12	5 (2%) 49 59	2, 6, 14, 23	0
1	B	175/194 (90%)	-0.14	2 (1%) 77 86	3, 6, 13, 24	0
1	C	175/194 (90%)	-0.11	3 (1%) 67 77	3, 7, 14, 24	0
1	D	175/194 (90%)	-0.04	4 (2%) 57 67	3, 7, 14, 24	0
All	All	700/776 (90%)	-0.10	14 (2%) 62 72	2, 6, 14, 24	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	THR	9.6
1	B	2	THR	7.4
1	A	2	THR	7.2
1	C	2	THR	5.5
1	C	102	PRO	5.3
1	B	3	LYS	5.1
1	D	176	LEU	4.6
1	D	3	LYS	4.6
1	A	102	PRO	3.4
1	D	101	HIS	2.7
1	A	3	LYS	2.5
1	A	101	HIS	2.4
1	C	101	HIS	2.3
1	A	104	ILE	2.2

### 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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BA	B	1177	1/1	0.08	-0.36	7,7,7,7	0
2	BA	D	1177	1/1	0.08	-0.40	5,5,5,5	0

### 6.5 Other polymers

There are no such residues in this entry.