



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 PM GMT

PDB ID : 4P6B
Title : Crystal structure of Est-Y29,a novel penicillin-binding protein/beta-lactamase homolog from a metagenomic library
Authors : Ngo, T.D.; Ryu, B.H.; Ju, H.S.; Jang, E.J.; Kim, K.K.; Kim, D.H.
Deposited on : 2014-03-24
Resolution : 1.70 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

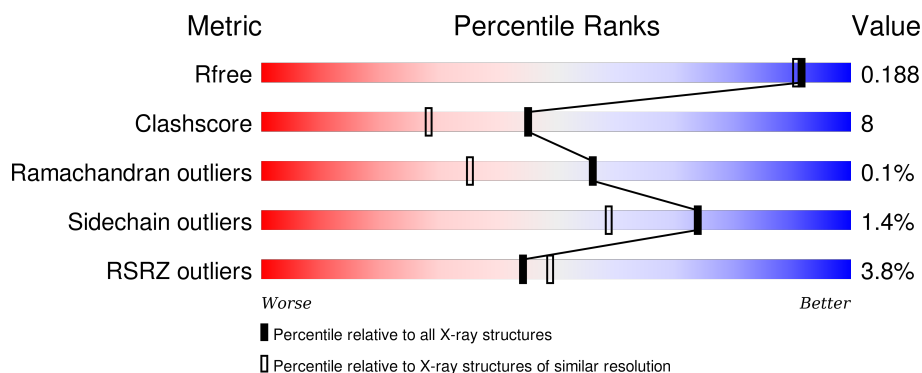
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 ≥ 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	390	<div> <div>5%</div> <div>90%</div> <div>8% ..</div> </div>
1	B	390	<div> <div>3%</div> <div>86%</div> <div>12% ..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6836 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 Est-Y29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2976	1899	501	554	22			
1	B	383	Total	C	N	O	S	0	0	0
			2962	1890	501	550	21			

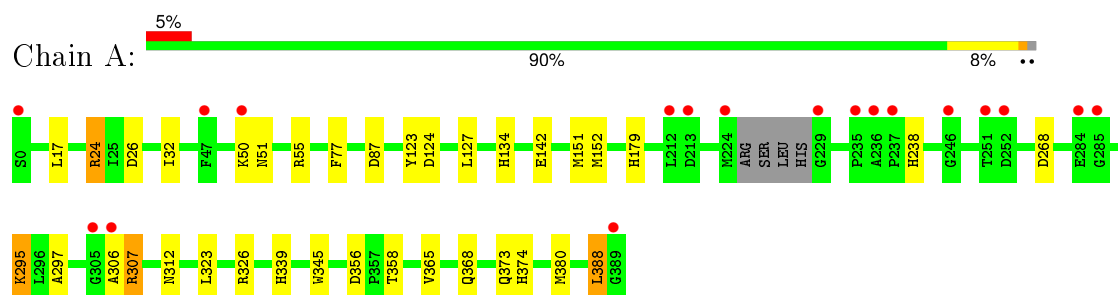
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	452	Total	O	0	0
			452	452		
2	B	446	Total	O	0	0
			446	446		

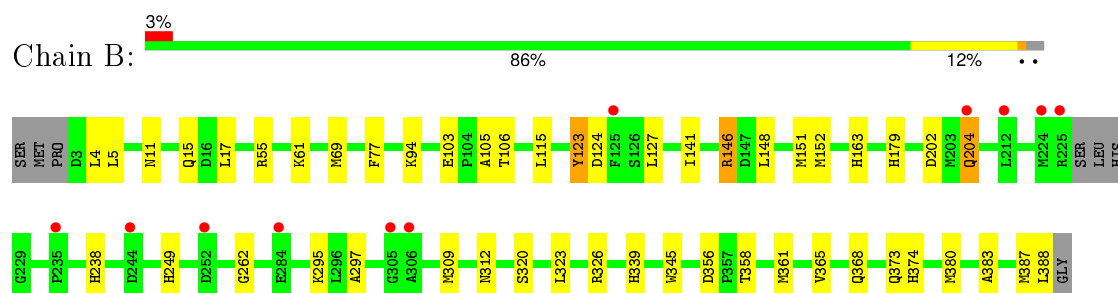
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Est-Y29



• Molecule 1: Est-Y29



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	121.54Å 121.54Å 155.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 28.65 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.70) 99.2 (28.65-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.91 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.170 , 0.188 0.170 , 0.188	Depositor DCC
R_{free} test set	6122 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.9	EDS
Estimated twinning fraction	0.016 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 122076 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6836	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.53	0/3052	0.65	4/4147 (0.1%)
1	B	0.52	0/3037	0.63	3/4126 (0.1%)
All	All	0.52	0/6089	0.64	7/8273 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	151	MET	CG-SD-CE	-6.68	89.51	100.20
1	B	146	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	295	LYS	CD-CE-NZ	5.94	125.36	111.70
1	A	326	ARG	CG-CD-NE	-5.45	100.35	111.80
1	A	24	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	326	ARG	CG-CD-NE	-5.15	100.98	111.80

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	2976	0	2906	33	0
1	B	2962	0	2892	58	0
2	A	452	0	0	7	1
2	B	446	0	0	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6836	0	5798	91	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 8.

All (91) 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:388:LEU:C	2:B:421:HOH:O	1.95	1.05
1:B:238:HIS:HD2	1:B:373:GLN:H	1.17	0.93
1:B:358:THR:HG21	2:B:747:HOH:O	1.72	0.90
1:A:238:HIS:HD2	1:A:373:GLN:H	1.16	0.90
1:B:202:ASP:OD1	1:B:204:GLN:NE2	2.07	0.87
1:B:5:LEU:HG	1:B:387:MET:CE	2.08	0.83
1:B:148:LEU:HD12	1:B:151:MET:HE1	1.61	0.83
1:B:5:LEU:HG	1:B:387:MET:HE3	1.69	0.74
1:B:339:HIS:HD2	1:B:356:ASP:OD2	1.70	0.74
1:B:106:THR:H	1:B:163:HIS:HD2	1.34	0.74
1:B:5:LEU:N	1:B:387:MET:HE1	2.04	0.72
1:A:339:HIS:HD2	1:A:356:ASP:OD2	1.72	0.72
1:A:55:ARG:H	1:A:368:GLN:HE22	1.38	0.71
1:B:148:LEU:HD12	1:B:151:MET:CE	2.21	0.70
1:A:358:THR:HG23	2:A:591:HOH:O	1.91	0.69
1:B:388:LEU:HD12	2:B:457:HOH:O	1.94	0.67
1:B:106:THR:H	1:B:163:HIS:CD2	2.12	0.67
1:A:238:HIS:CD2	1:A:373:GLN:H	2.07	0.67
1:B:55:ARG:H	1:B:368:GLN:HE22	1.44	0.66
1:B:17:LEU:O	1:B:238:HIS:HE1	1.79	0.66
1:B:5:LEU:HG	1:B:387:MET:HE1	1.78	0.65
1:A:87:ASP:OD1	1:A:179:HIS:HE1	1.78	0.65
1:A:127:LEU:H	1:A:312:ASN:HD21	1.44	0.65
1:B:127:LEU:H	1:B:312:ASN:HD21	1.44	0.64
1:B:61:LYS:NZ	2:B:550:HOH:O	2.31	0.64
1:B:262:GLY:O	2:B:680:HOH:O	2.15	0.63
1:A:134:HIS:HD2	2:A:514:HOH:O	1.82	0.62
1:A:17:LEU:O	1:A:238:HIS:HE1	1.81	0.62
1:B:146:ARG:HD2	2:B:518:HOH:O	1.99	0.62
1:B:238:HIS:CD2	1:B:373:GLN:H	2.09	0.62
1:A:55:ARG:H	1:A:368:GLN:NE2	1.98	0.61
1:B:4:LEU:HB2	1:B:387:MET:HE2	1.82	0.61
1:B:146:ARG:HD3	1:B:151:MET:HA	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:HIS:HE1	2:B:511:HOH:O	1.83	0.60
1:B:361:MET:HE2	1:B:388:LEU:HD11	1.84	0.59
1:B:55:ARG:H	1:B:368:GLN:NE2	2.00	0.59
1:A:306:ALA:O	1:A:307:ARG:HB2	2.03	0.59
1:B:383:ALA:O	1:B:387:MET:HE2	2.03	0.59
1:A:373:GLN:HG3	2:A:732:HOH:O	2.02	0.58
1:B:148:LEU:CD1	1:B:151:MET:HE1	2.32	0.58
1:A:55:ARG:HH11	1:A:368:GLN:HE21	1.53	0.56
1:B:11:ASN:HD21	1:B:15:GLN:HE21	1.52	0.56
1:B:146:ARG:HD3	1:B:151:MET:CA	2.35	0.56
1:B:5:LEU:H	1:B:387:MET:HE1	1.69	0.56
1:A:24:ARG:CD	1:A:26:ASP:OD1	2.53	0.56
1:A:24:ARG:HD3	1:A:26:ASP:OD1	2.06	0.55
1:B:11:ASN:HD21	1:B:15:GLN:NE2	2.03	0.55
1:A:295:LYS:HE3	2:A:794:HOH:O	2.06	0.54
1:A:24:ARG:NH2	1:A:268:ASP:OD1	2.40	0.54
1:B:69:MET:HE3	1:B:115:LEU:HD13	1.89	0.53
1:A:179:HIS:HD2	2:A:548:HOH:O	1.90	0.53
1:A:374:HIS:HE1	2:A:791:HOH:O	1.91	0.53
1:B:69:MET:CE	1:B:115:LEU:CD1	2.87	0.53
1:B:361:MET:CE	1:B:388:LEU:HD11	2.39	0.52
1:B:4:LEU:HB2	1:B:387:MET:CE	2.39	0.52
1:B:69:MET:HE3	1:B:115:LEU:CD1	2.39	0.52
1:B:152:MET:HG3	1:B:179:HIS:CG	2.45	0.52
1:B:55:ARG:HH11	1:B:368:GLN:HE21	1.59	0.51
1:B:69:MET:HE1	1:B:115:LEU:HD11	1.93	0.48
1:A:32:ILE:CD1	1:A:388:LEU:HD11	2.43	0.48
1:A:32:ILE:HD11	1:A:388:LEU:HD21	1.95	0.48
1:B:146:ARG:NH2	2:B:733:HOH:O	2.38	0.48
1:B:105:ALA:HA	1:B:163:HIS:CD2	2.49	0.47
1:A:55:ARG:HH11	1:A:368:GLN:NE2	2.13	0.47
1:A:345:TRP:CE3	1:A:345:TRP:HA	2.50	0.47
1:B:345:TRP:CE3	1:B:345:TRP:HA	2.49	0.47
1:B:69:MET:CE	1:B:115:LEU:HD13	2.44	0.47
1:B:69:MET:CE	1:B:115:LEU:HD11	2.46	0.46
1:B:374:HIS:HE1	2:B:663:HOH:O	1.99	0.45
1:A:152:MET:HG3	1:A:179:HIS:CG	2.51	0.45
1:A:365:VAL:HG21	1:A:380:MET:HB2	1.97	0.45
1:B:365:VAL:HG21	1:B:380:MET:HB2	1.98	0.45
1:B:297:ALA:HA	1:B:323:LEU:HD12	1.99	0.45
1:A:24:ARG:HD2	1:A:26:ASP:OD1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ALA:C	1:B:387:MET:CE	2.86	0.44
1:B:146:ARG:HD3	1:B:151:MET:HB2	1.99	0.44
1:B:383:ALA:O	1:B:387:MET:CE	2.65	0.44
1:B:103:GLU:OE2	1:B:163:HIS:HE1	2.00	0.43
1:B:309:MET:HE1	1:B:320:SER:O	2.18	0.43
1:B:123:TYR:CD1	1:B:141:ILE:HD11	2.53	0.43
1:A:32:ILE:HD12	1:A:388:LEU:HD11	2.01	0.43
1:B:94:LYS:NZ	2:B:830:HOH:O	2.50	0.43
1:A:365:VAL:HG21	1:A:380:MET:CB	2.49	0.43
1:B:55:ARG:HH11	1:B:368:GLN:NE2	2.17	0.42
1:A:50:LYS:HE2	1:A:51:ASN:HD21	1.84	0.42
1:A:297:ALA:HA	1:A:323:LEU:HD12	2.01	0.42
1:B:339:HIS:CD2	1:B:356:ASP:OD2	2.61	0.42
1:B:69:MET:HE1	1:B:115:LEU:CD1	2.49	0.41
1:A:306:ALA:O	1:A:307:ARG:CB	2.66	0.41
1:A:142:GLU:HG2	2:A:785:HOH:O	2.21	0.41
1:A:87:ASP:OD1	1:A:179:HIS:CE1	2.66	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:472:HOH:O	2:B:467:HOH:O[3_655]	2.14	0.06

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	382/390 (98%)	372 (97%)	9 (2%)	1 (0%)	46	26
1	B	379/390 (97%)	369 (97%)	10 (3%)	0	100	100
All	All	761/780 (98%)	741 (97%)	19 (2%)	1 (0%)	56	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ARG

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	316/321 (98%)	312 (99%)	4 (1%)	76	62
1	B	314/321 (98%)	309 (98%)	5 (2%)	70	54
All	All	630/642 (98%)	621 (99%)	9 (1%)	74	59

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

Mol	Chain	Res	Type
1	A	77	PHE
1	A	123	TYR
1	A	124	ASP
1	A	388	LEU
1	B	77	PHE
1	B	123	TYR
1	B	124	ASP
1	B	204	GLN
1	B	295	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	134	HIS
1	A	179	HIS
1	A	238	HIS
1	A	275	ASN
1	A	303	HIS
1	A	312	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	339	HIS
1	A	368	GLN
1	A	374	HIS
1	B	15	GLN
1	B	163	HIS
1	B	238	HIS
1	B	249	HIS
1	B	275	ASN
1	B	312	ASN
1	B	339	HIS
1	B	368	GLN
1	B	374	HIS

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, 95th 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 ²)	Q<0.9
1	A	386/390 (98%)	0.05	18 (4%) 35 39	9, 16, 29, 35	0
1	B	383/390 (98%)	-0.05	11 (2%) 55 59	10, 16, 28, 42	0
All	All	769/780 (98%)	0.00	29 (3%) 44 49	9, 16, 29, 42	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ALA	8.2
1	B	306	ALA	5.9
1	B	212	LEU	5.1
1	A	0	SER	4.7
1	A	252	ASP	4.6
1	B	305	GLY	4.0
1	A	305	GLY	3.9
1	B	284	GLU	3.8
1	A	237	PRO	3.5
1	B	252	ASP	3.4
1	A	213	ASP	3.3
1	A	47	PHE	3.0
1	A	229	GLY	2.9
1	A	224	MET	2.8
1	A	284	GLU	2.8
1	B	125	PHE	2.7
1	B	235	PRO	2.7
1	A	251	THR	2.7
1	B	224	MET	2.6
1	A	50	LYS	2.6
1	A	246	GLY	2.6
1	A	236	ALA	2.5
1	A	285	GLY	2.4
1	B	225	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	204	GLN	2.4
1	A	235	PRO	2.2
1	B	244	ASP	2.1
1	A	389	GLY	2.1
1	A	212	LEU	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.