WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2022 – 06:04 PM JST

PDB ID	:	6IV0
Title	:	Crystal structure of a bacterial Bestrophin homolog from Klebsiella pneumoniae with a mutation I180A
Authors	:	Kittredge, A.; Chen, S.; Yang, T.
Deposited on	:	2018-12-02
Resolution	:	2.90 Å(reported)

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

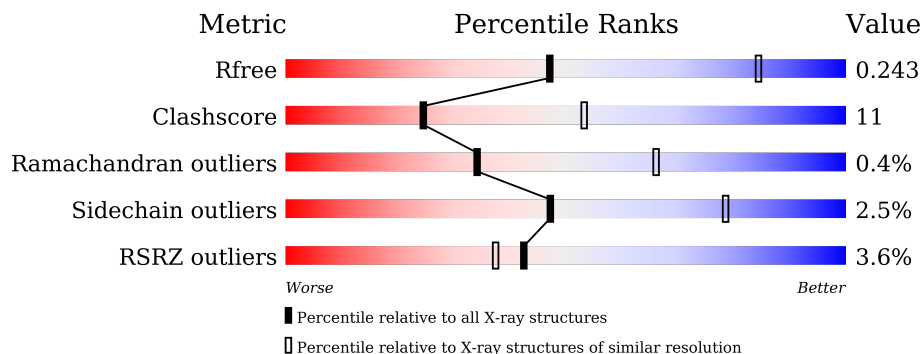|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.90 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		11
Ramachandran outliers		0.4%
Sidechain outliers		2.5%
RSRZ outliers		3.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	296	3% 69% 20% • 9%
1	B	296	3% 67% 23% • 9%
1	C	296	4% 74% 16% • 9%
1	D	296	2% 63% 27% • 9%
1	E	296	4% 71% 18% • 9%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10621 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 Bestrophin homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2104	1363	353	379	9			
1	B	270	Total	C	N	O	S	0	0	0
			2139	1382	364	384	9			
1	C	269	Total	C	N	O	S	0	0	0
			2101	1353	362	377	9			
1	D	268	Total	C	N	O	S	0	0	0
			2111	1364	359	379	9			
1	E	270	Total	C	N	O	S	0	0	0
			2127	1374	364	380	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP W1ELP7
A	0	ALA	-	expression tag	UNP W1ELP7
A	180	ALA	ILE	engineered mutation	UNP W1ELP7
B	-1	ASN	-	expression tag	UNP W1ELP7
B	0	ALA	-	expression tag	UNP W1ELP7
B	180	ALA	ILE	engineered mutation	UNP W1ELP7
C	-1	ASN	-	expression tag	UNP W1ELP7
C	0	ALA	-	expression tag	UNP W1ELP7
C	180	ALA	ILE	engineered mutation	UNP W1ELP7
D	-1	ASN	-	expression tag	UNP W1ELP7
D	0	ALA	-	expression tag	UNP W1ELP7
D	180	ALA	ILE	engineered mutation	UNP W1ELP7
E	-1	ASN	-	expression tag	UNP W1ELP7
E	0	ALA	-	expression tag	UNP W1ELP7
E	180	ALA	ILE	engineered mutation	UNP W1ELP7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Zn 4	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	3	Total 3	Zn 3	0	0
2	D	4	Total 4	Zn 4	0	0
2	E	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

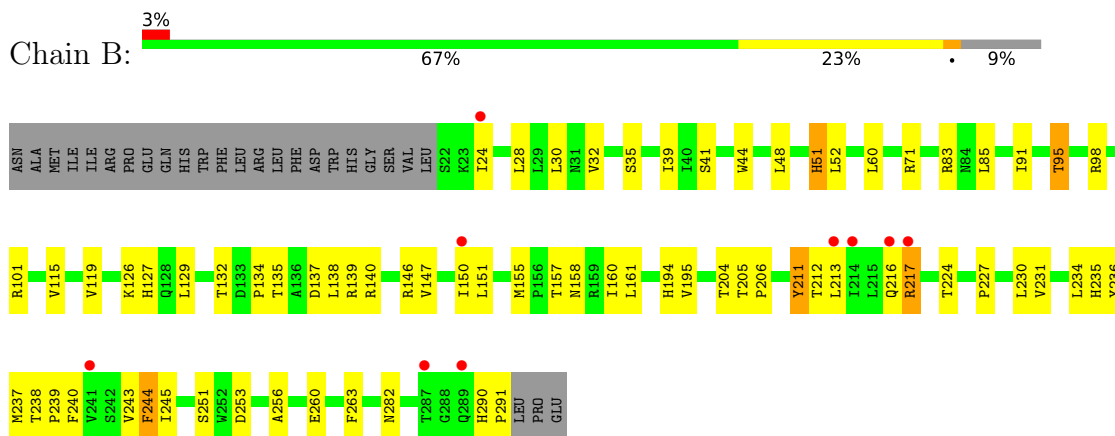| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	4	Total 4	O 4	0	0
3	C	6	Total 6	O 6	0	0
3	D	3	Total 3	O 3	0	0
3	E	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
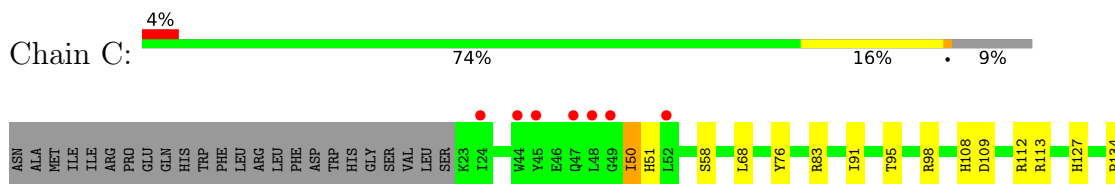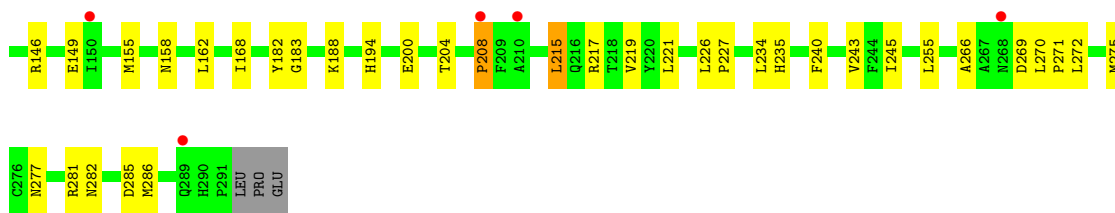
- Molecule 1: Bestrophin homolog
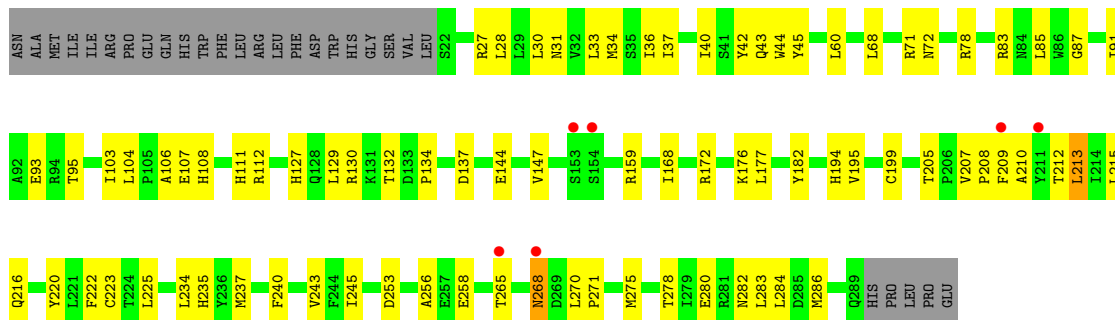
Chain A:

- Molecule 1: Bestrophin homolog

Chain B:

- Molecule 1: Bestrophin homolog

Chain C:

R146 E149 I150 M155 N158 L162 I168 Y182 G183 K188 H194 E200 T204 P208 F209 A210 L215 Q216 R217 T218 V219 Y220 L221 L226 P227 L234 H235 F240 V243 F244 I245 L255 A266 A267 N268 D269 L270 P271 L272 M275

C276 N277 R281 N282 D285 M286 Q289 H290 P291 LEU PRO GLU

• Molecule 1: Bestrophin homolog

Chain D:

ASN ALA MET ILE ARG PRO GLU GLN HIS TRP PHE LEU ARG LEU PHE ASP TRP HIS GLY SER VAL LEU S22 R27 L28 L29 L30 N31 V32 L33 M34 S35 I36 I37 I40 S41 Y42 Q43 W44 Y45 L60 L68 R71 N72 R78 R83 N84 L85 W86 G87 I91

A92 E93 R94 T95 I103 L104 P105 A106 E107 H108 H111 R112 H127 Q128 L129 R130 K131 T132 D133 P134 D137 E144 V147 S153 S154 R159 I168 R172 K176 L177 Y182 H194 V195 C199 T205 P206 V207 F209 A210 Y211 T212 L213 I214 L215

Q216 Y220 L221 F222 C223 T224 L225 L234 H235 Y236 M237 F240 V243 F244 I245 D253 A256 E257 E258 T265 N268 D269 L270 P271 M275 T278 I279 E280 R281 N282 L283 L284 D285 M286 Q289 HIS PRO LEU PRO GLU

• Molecule 1: Bestrophin homolog

Chain E:

ASN ALA MET ILE ILE ARG PRO GLU GLN HIS TRP PHE LEU ARG LEU PHE ASP TRP HIS GLY SER VAL LEU SER LYS I24 I25 F26 R27 N31 I40 S41 Y42 Q43 W44 Y45 E46 Q47 L48 G49 I50 H51 L52 T53 V54 A55 P56 F57 L60 S77 G87 T88 V89 L90 I91

A92 E93 R94 V97 R98 Q99 L100 R113 I114 V115 S116 R130 K131 R139 E144 E145 R146 E149 M155 L184 K188 E191 H194 V195 R201 T204 T205 P206 V207 P208 Y211 Y220 L221 F222 C223 L226 A229 L230 V231 Y236 L259

T265 A266 A267 N268 D269 L270 P271 L272 L283 Q289 H290 P293 GLU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.57Å 159.91Å 161.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.38 – 2.90 65.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.38-2.90) 99.9 (65.38-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.201 , 0.238 0.209 , 0.243	Depositor DCC
R_{free} test set	1995 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.1	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10621	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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

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	0.50	0/2149	0.65	0/2929
1	B	0.51	0/2187	0.65	0/2979
1	C	0.47	0/2146	0.61	0/2925
1	D	0.47	0/2156	0.63	0/2937
1	E	0.52	0/2173	0.66	1/2961 (0.0%)
All	All	0.49	0/10811	0.64	1/14731 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	206	PRO	N-CA-C	-6.91	94.14	112.10

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	2104	0	2122	54	0
1	B	2139	0	2160	62	0
1	C	2101	0	2110	41	0
1	D	2111	0	2138	58	0
1	E	2127	0	2162	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
3	C	6	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
All	All	10621	0	10692	231	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 11.

The worst 5 of 231 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:C:68:LEU:HD23	1:C:215:LEU:CD1	1.77	1.13
1:D:212:THR:HG22	1:D:216:GLN:HE22	1.21	1.05
1:E:207:VAL:HG23	1:E:208:PRO:HD3	1.32	1.04
1:C:68:LEU:CD2	1:C:215:LEU:CD1	2.47	0.93
1:B:212:THR:HG22	1:B:216:GLN:NE2	1.84	0.91

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	266/296 (90%)	254 (96%)	10 (4%)	2 (1%)	19	51
1	B	268/296 (90%)	241 (90%)	27 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	267/296 (90%)	249 (93%)	17 (6%)	1 (0%)	34	66
1	D	266/296 (90%)	252 (95%)	13 (5%)	1 (0%)	34	66
1	E	268/296 (90%)	255 (95%)	12 (4%)	1 (0%)	34	66
All	All	1335/1480 (90%)	1251 (94%)	79 (6%)	5 (0%)	34	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	208	PRO
1	A	44	TRP
1	A	40	ILE
1	D	40	ILE
1	E	208	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	225/258 (87%)	221 (98%)	4 (2%)	59	85
1	B	231/258 (90%)	222 (96%)	9 (4%)	32	66
1	C	223/258 (86%)	220 (99%)	3 (1%)	69	90
1	D	227/258 (88%)	224 (99%)	3 (1%)	69	90
1	E	230/258 (89%)	221 (96%)	9 (4%)	32	66
All	All	1136/1290 (88%)	1108 (98%)	28 (2%)	47	78

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	58	SER
1	E	207	VAL
1	D	225	LEU
1	E	130	ARG
1	D	213	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	47	GLN
1	E	235	HIS
1	E	290	HIS
1	D	268	ASN
1	D	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 15 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.

No monomer is involved in short contacts.

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, 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	268/296 (90%)	0.06	9 (3%)	45	40	46, 69, 119, 141	0
1	B	270/296 (91%)	0.04	9 (3%)	46	41	49, 77, 115, 133	0
1	C	269/296 (90%)	0.03	12 (4%)	33	29	51, 75, 128, 149	0
1	D	268/296 (90%)	-0.05	6 (2%)	62	59	52, 86, 120, 130	0
1	E	270/296 (91%)	0.14	13 (4%)	30	27	46, 70, 120, 146	0
All	All	1345/1480 (90%)	0.04	49 (3%)	42	37	46, 76, 121, 149	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	204	THR	5.4
1	A	289	GLN	5.2
1	E	48	LEU	4.5
1	E	265	THR	4.5
1	A	40	ILE	4.4

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 monosaccharides 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. The B-factors column lists the minimum,

median, 95th 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	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	ZN	D	303	1/1	0.20	0.24	117,117,117,117	0
2	ZN	B	301	1/1	0.86	0.11	133,133,133,133	0
2	ZN	D	304	1/1	0.89	0.13	128,128,128,128	0
2	ZN	C	302	1/1	0.94	0.15	76,76,76,76	0
2	ZN	D	302	1/1	0.94	0.16	87,87,87,87	0
2	ZN	E	302	1/1	0.95	0.20	71,71,71,71	0
2	ZN	B	302	1/1	0.97	0.19	73,73,73,73	0
2	ZN	A	304	1/1	0.97	0.12	80,80,80,80	0
2	ZN	A	303	1/1	0.97	0.14	81,81,81,81	0
2	ZN	A	302	1/1	0.98	0.20	76,76,76,76	0
2	ZN	A	301	1/1	0.98	0.15	74,74,74,74	0
2	ZN	C	303	1/1	0.99	0.16	75,75,75,75	0
2	ZN	E	301	1/1	0.99	0.17	63,63,63,63	0
2	ZN	D	301	1/1	0.99	0.15	76,76,76,76	0
2	ZN	C	301	1/1	1.00	0.22	69,69,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK