



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:49 PM UTC

PDB ID : 1AUO / pdb_00001auo
Title : CARBOXYLESTERASE FROM PSEUDOMONAS FLUORESCENS
Authors : Kim, K.K.; Song, H.K.; Suh, S.W.
Deposited on : 1997-09-01
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

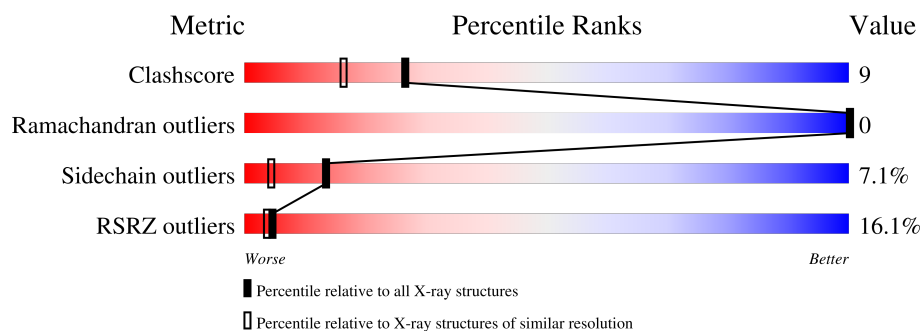
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 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 $\leq 5\%$. 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	218	7% 81% 17% .
1	B	218	25% 68% 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3599 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 CARBOXYLESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1682	1075	285	313	9			
1	B	218	Total	C	N	O	S	0	0	0
			1682	1075	285	313	9			

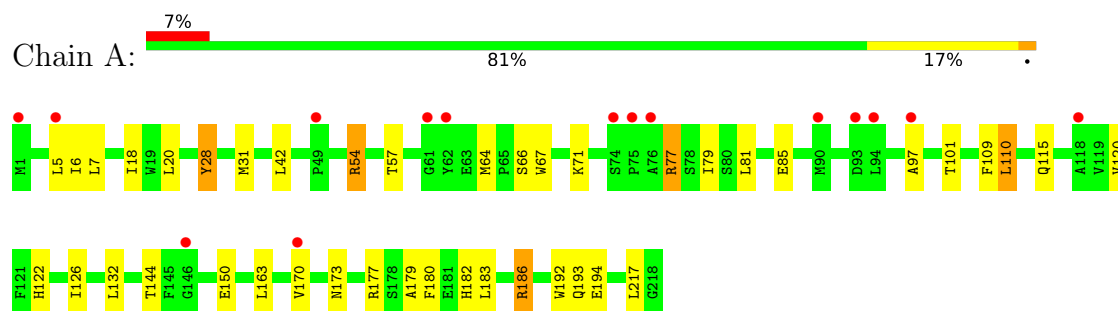
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	136	Total	O	0	0
			136	136		
2	B	99	Total	O	0	0
			99	99		

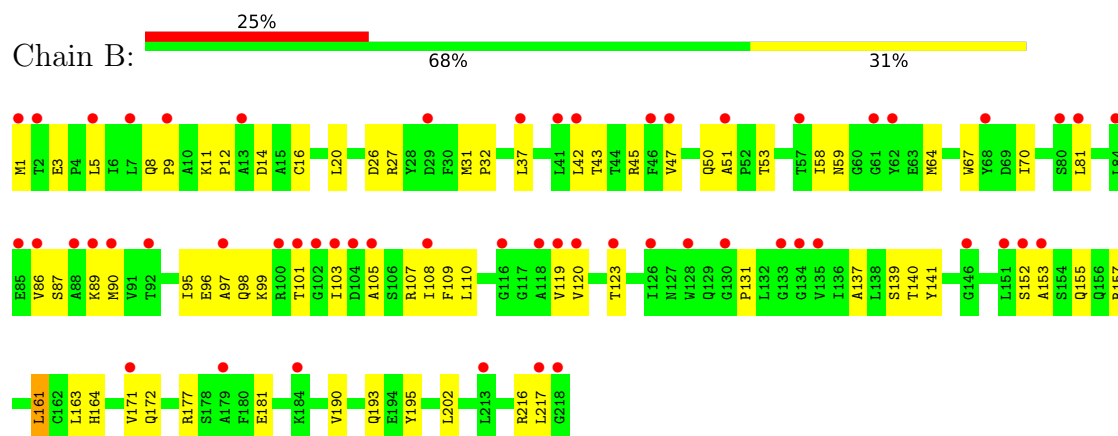
3 Residue-property plots

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: CARBOXYLESTERASE



• Molecule 1: CARBOXYLESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.04Å 82.04Å 145.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80 8.00 – 1.81	Depositor EDS
% Data completeness (in resolution range)	91.0 (8.00-1.80) 89.5 (8.00-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.81Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.208 , 0.273 0.303 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3599	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.93	1/1725 (0.1%)	1.06	6/2349 (0.3%)
1	B	0.66	0/1725	0.90	2/2349 (0.1%)
All	All	0.80	1/3450 (0.0%)	0.98	8/4698 (0.2%)

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	A	0	4
1	B	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	ALA	CA-CB	5.55	1.62	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	LEU	CA-C-N	6.42	127.87	119.84
1	B	202	LEU	C-N-CA	6.42	127.87	119.84
1	A	57	THR	N-CA-C	5.93	118.23	111.11
1	A	183	LEU	N-CA-C	-5.29	105.10	112.45
1	A	170	VAL	N-CA-C	-5.19	107.10	111.56
1	A	79	ILE	N-CA-C	5.16	117.47	108.95
1	A	64	MET	CA-C-N	-5.12	114.52	119.90
1	A	64	MET	C-N-CA	-5.12	114.52	119.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Sidechain
1	A	28	TYR	Sidechain
1	A	6	ILE	Mainchain
1	A	97	ALA	Mainchain
1	B	141	TYR	Sidechain
1	B	181	GLU	Mainchain

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	1682	0	1658	20	0
1	B	1682	0	1658	42	1
2	A	136	0	0	1	1
2	B	99	0	0	4	0
All	All	3599	0	3316	62	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 9.

All (62) 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:A:77:ARG:H	1:A:77:ARG:HD3	1.40	0.86
1:B:171:VAL:HB	2:B:1287:HOH:O	1.79	0.83
1:B:26:ASP:HB2	1:B:50:GLN:NE2	2.03	0.74
1:B:161:LEU:HD13	1:B:163:LEU:HD11	1.70	0.72
1:A:182:HIS:HD2	1:A:186:ARG:HH12	1.35	0.72
1:B:105:ALA:HA	1:B:108:ILE:HD12	1.72	0.71
1:B:27:ARG:H	1:B:50:GLN:HE21	1.40	0.69
1:B:103:ILE:HG12	2:B:1186:HOH:O	1.92	0.69
1:A:173:ASN:HD21	1:A:194:GLU:CD	2.05	0.64
1:B:123:THR:HG22	2:B:1120:HOH:O	1.98	0.63
1:B:105:ALA:HB3	1:B:131:PRO:HB2	1.79	0.63
1:A:67:TRP:H	1:A:115:GLN:NE2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:SER:H	1:B:155:GLN:NE2	2.01	0.58
1:B:45:ARG:HH21	1:B:103:ILE:HD11	1.69	0.58
1:B:137:ALA:HB1	1:B:140:THR:CG2	2.34	0.58
1:A:122:HIS:HD2	1:A:144:THR:OG1	1.87	0.57
1:A:54:ARG:HD3	1:A:66:SER:O	2.05	0.56
1:B:58:ILE:HG23	1:B:70:ILE:O	2.06	0.56
1:A:182:HIS:CD2	1:A:186:ARG:HH12	2.21	0.55
1:A:81:LEU:O	1:A:85:GLU:HG3	2.05	0.55
1:B:14:ASP:O	1:B:107:ARG:HD3	2.06	0.55
1:A:180:PHE:CE2	1:A:192:TRP:HB2	2.44	0.53
1:B:11:LYS:HB2	1:B:43:THR:HG22	1.91	0.53
1:B:152:SER:H	1:B:155:GLN:HE21	1.58	0.52
1:B:86:VAL:HG23	2:B:1198:HOH:O	2.09	0.52
1:B:139:SER:O	1:B:171:VAL:HG21	2.11	0.51
1:B:153:ALA:O	1:B:157:ARG:HG3	2.10	0.51
1:B:8:GLN:OE1	1:B:45:ARG:HD3	2.11	0.50
1:A:5:LEU:HD11	1:A:28:TYR:CD1	2.47	0.49
1:A:122:HIS:O	1:A:126:ILE:HB	2.13	0.49
1:B:45:ARG:NH2	1:B:103:ILE:HD11	2.26	0.49
1:A:77:ARG:HB3	2:A:1231:HOH:O	2.12	0.48
1:B:109:PHE:HE1	1:B:217:LEU:HD21	1.78	0.48
1:B:20:LEU:N	1:B:20:LEU:HD12	2.29	0.48
1:B:216:ARG:HH11	1:B:216:ARG:HG2	1.78	0.47
1:B:110:LEU:HB3	1:B:120:VAL:HG13	1.96	0.47
1:A:110:LEU:HB3	1:A:120:VAL:HG13	1.97	0.46
1:A:7:LEU:HD11	1:A:31:MET:HG3	1.98	0.45
1:A:20:LEU:HD12	1:A:20:LEU:N	2.32	0.44
1:B:171:VAL:HG23	1:B:171:VAL:O	2.17	0.44
1:A:110:LEU:HD22	1:A:132:LEU:HD21	2.00	0.44
1:B:59:ASN:HD22	1:B:64:MET:CE	2.31	0.44
1:B:16:CYS:HB2	1:B:103:ILE:HD13	2.00	0.43
1:B:163:LEU:HD23	1:B:195:TYR:CE2	2.52	0.43
1:A:217:LEU:HA	1:A:217:LEU:HD23	1.81	0.43
1:B:11:LYS:HB3	1:B:12:PRO:HD2	2.00	0.43
1:B:51:ALA:HB2	1:B:67:TRP:CE2	2.54	0.43
1:B:9:PRO:HB2	1:B:42:LEU:O	2.19	0.42
1:B:11:LYS:HE3	1:B:43:THR:CG2	2.49	0.42
1:B:27:ARG:HB3	1:B:50:GLN:HB2	2.00	0.42
1:B:216:ARG:HA	1:B:216:ARG:HD3	1.67	0.42
1:B:97:ALA:O	1:B:101:THR:HG23	2.20	0.42
1:B:67:TRP:HE3	1:B:87:SER:OG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HD23	1:B:195:TYR:HE2	1.84	0.41
1:B:98:GLN:HB3	1:B:103:ILE:HD12	2.01	0.41
1:B:67:TRP:HB3	1:B:119:VAL:HG21	2.02	0.41
1:A:109:PHE:HE1	1:A:217:LEU:HD21	1.86	0.41
1:B:95:ILE:HD11	1:B:110:LEU:HD11	2.02	0.41
1:B:31:MET:HB3	1:B:32:PRO:HD3	2.03	0.41
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.76	0.40
1:A:122:HIS:CD2	1:A:126:ILE:HD12	2.57	0.40
1:A:18:ILE:HB	1:A:110:LEU:HD12	2.04	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)
1:B:53:THR:OG1	2:A:1201:HOH:O[6_555]	2.13	0.07

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	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
1	B	216/218 (99%)	213 (99%)	3 (1%)	0	100	100
All	All	432/436 (99%)	420 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	176/176 (100%)	166 (94%)	10 (6%)	18	8
1	B	176/176 (100%)	161 (92%)	15 (8%)	10	3
All	All	352/352 (100%)	327 (93%)	25 (7%)	13	4

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	54	ARG
1	A	71	LYS
1	A	77	ARG
1	A	101	THR
1	A	110	LEU
1	A	150	GLU
1	A	163	LEU
1	A	177	ARG
1	A	193	GLN
1	B	1	MET
1	B	3	GLU
1	B	5	LEU
1	B	47	VAL
1	B	81	LEU
1	B	89	LYS
1	B	90	MET
1	B	96	GLU
1	B	99	LYS
1	B	161	LEU
1	B	164	HIS
1	B	172	GLN
1	B	177	ARG
1	B	190	VAL
1	B	193	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	115	GLN

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Mol	Chain	Res	Type
1	A	122	HIS
1	A	127	ASN
1	A	166	GLN
1	A	173	ASN
1	A	182	HIS
1	B	38	GLN
1	B	50	GLN
1	B	98	GLN
1	B	122	HIS
1	B	127	ASN
1	B	155	GLN
1	B	156	GLN
1	B	164	HIS
1	B	173	ASN
1	B	182	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 oligosaccharides 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	218/218 (100%)	0.96	15 (6%)	23 21	12, 21, 38, 65	0
1	B	218/218 (100%)	1.54	55 (25%)	1 1	18, 35, 53, 82	0
All	All	436/436 (100%)	1.25	70 (16%)	4 4	12, 29, 51, 82	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	GLY	5.4
1	B	86	VAL	4.9
1	B	97	ALA	4.8
1	B	1	MET	4.6
1	B	103	ILE	3.9
1	A	75	PRO	3.5
1	B	88	ALA	3.4
1	B	2	THR	3.4
1	B	100	ARG	3.4
1	B	130	GLY	3.3
1	B	171	VAL	3.3
1	B	61	GLY	3.3
1	B	13	ALA	3.3
1	B	152	SER	3.3
1	A	1	MET	3.2
1	B	90	MET	3.1
1	B	128	TRP	3.0
1	B	126	ILE	2.9
1	B	41	LEU	2.9
1	B	102	GLY	2.9
1	B	153	ALA	2.9
1	B	81	LEU	2.9
1	B	119	VAL	2.9
1	A	62	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	9	PRO	2.9
1	B	217	LEU	2.8
1	B	101	THR	2.7
1	A	90	MET	2.7
1	B	80	SER	2.7
1	B	5	LEU	2.6
1	B	57	THR	2.6
1	B	92	THR	2.6
1	A	5	LEU	2.5
1	B	104	ASP	2.5
1	B	179	ALA	2.5
1	A	94	LEU	2.5
1	B	84	LEU	2.4
1	B	213	LEU	2.4
1	B	146	GLY	2.4
1	B	51	ALA	2.4
1	A	146	GLY	2.4
1	B	42	LEU	2.3
1	A	118	ALA	2.3
1	B	46	PHE	2.3
1	B	85	GLU	2.3
1	B	120	VAL	2.3
1	B	151	LEU	2.3
1	A	49	PRO	2.2
1	B	134	GLY	2.2
1	A	93	ASP	2.2
1	B	135	VAL	2.2
1	B	7	LEU	2.2
1	B	68	TYR	2.2
1	B	89	LYS	2.2
1	B	29	ASP	2.2
1	A	74	SER	2.2
1	B	133	GLY	2.2
1	B	47	VAL	2.1
1	B	123	THR	2.1
1	A	61	GLY	2.1
1	B	116	GLY	2.1
1	B	105	ALA	2.1
1	B	118	ALA	2.1
1	A	76	ALA	2.1
1	A	97	ALA	2.1
1	B	37	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	184	LYS	2.0
1	B	108	ILE	2.0
1	B	62	TYR	2.0
1	A	170	VAL	2.0

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 oligosaccharides 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.