



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:59 PM UTC

PDB ID : 2Z5L / pdb_00002z5l
Title : The first ketoreductase of the tylosin PKS
Authors : Keatinge-Clay, A.T.; Stroud, R.M.
Deposited on : 2007-07-14
Resolution : 1.95 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

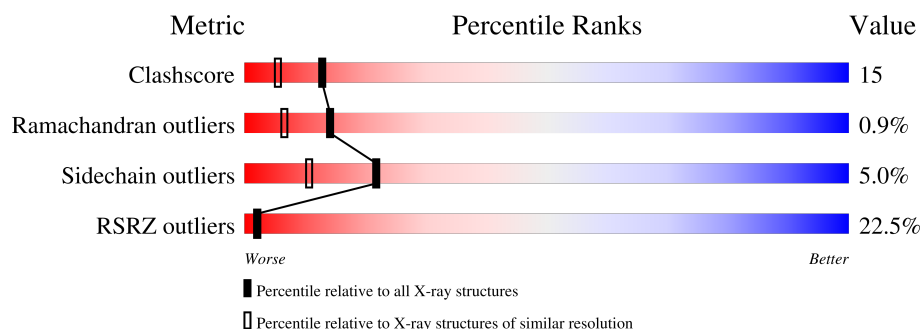
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	511	20% 63% 23% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3406 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 Ty lactone synthase starter module and modules 1 & 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3303	2055	609	629	10			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP O33954
A	-19	GLY	-	expression tag	UNP O33954
A	-18	SER	-	expression tag	UNP O33954
A	-17	SER	-	expression tag	UNP O33954
A	-16	HIS	-	expression tag	UNP O33954
A	-15	HIS	-	expression tag	UNP O33954
A	-14	HIS	-	expression tag	UNP O33954
A	-13	HIS	-	expression tag	UNP O33954
A	-12	HIS	-	expression tag	UNP O33954
A	-11	HIS	-	expression tag	UNP O33954
A	-10	SER	-	expression tag	UNP O33954
A	-9	SER	-	expression tag	UNP O33954
A	-8	GLY	-	expression tag	UNP O33954
A	-7	LEU	-	expression tag	UNP O33954
A	-6	VAL	-	expression tag	UNP O33954
A	-5	PRO	-	expression tag	UNP O33954
A	-4	ARG	-	expression tag	UNP O33954
A	-3	GLY	-	expression tag	UNP O33954
A	-2	SER	-	expression tag	UNP O33954
A	-1	HIS	-	expression tag	UNP O33954
A	0	MET	-	expression tag	UNP O33954

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total	O	0	0
			103	103		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.18Å 49.81Å 68.81Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 50.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.4 (50.00-1.95) 82.1 (50.00-1.96)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.97Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.287 0.271 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3406	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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 [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	0.45	0/3357	0.91	3/4575 (0.1%)

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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	293	VAL	N-CA-C	8.07	119.41	108.11
1	A	459	VAL	N-CA-C	6.28	117.81	108.46
1	A	56	VAL	N-CA-C	5.36	116.50	109.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	413	GLY	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	3303	0	3308	100	0
2	A	103	0	0	7	0
All	All	3406	0	3308	100	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 15.

All (100) 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:126:ARG:HH21	1:A:127:ARG:HD3	1.28	0.95
1:A:63:ILE:HD11	1:A:95:VAL:HG21	1.56	0.87
1:A:46:THR:HG22	1:A:56:VAL:HG11	1.64	0.79
1:A:30:LEU:HD12	1:A:57:ALA:O	1.84	0.77
1:A:343:GLY:O	1:A:347:CYS:HB2	1.86	0.76
1:A:431:LEU:HD23	1:A:459:VAL:HG13	1.67	0.75
1:A:249:ALA:HB3	1:A:417:MET:SD	2.27	0.75
1:A:63:ILE:HD13	1:A:95:VAL:HG11	1.72	0.69
1:A:271:ARG:HG2	2:A:544:HOH:O	1.93	0.68
1:A:344:ALA:HB3	2:A:590:HOH:O	1.92	0.68
1:A:78:MET:HE3	1:A:116:VAL:HG11	1.74	0.68
1:A:126:ARG:NH2	1:A:127:ARG:HD3	2.07	0.67
1:A:455:THR:HG22	1:A:457:VAL:HG23	1.78	0.66
1:A:324:ILE:CD1	1:A:340:THR:HG22	2.27	0.64
1:A:76:PRO:HG2	2:A:540:HOH:O	1.99	0.61
1:A:365:PHE:HB3	1:A:404:ALA:HA	1.82	0.60
1:A:74:LEU:HD11	1:A:107:LEU:HD12	1.84	0.60
1:A:271:ARG:NH1	2:A:492:HOH:O	2.36	0.59
1:A:429:ARG:O	1:A:464:PHE:HA	2.03	0.59
1:A:50:SER:C	1:A:52:ARG:H	2.11	0.58
1:A:247:MET:HE1	1:A:279:ALA:HA	1.84	0.58
1:A:247:MET:HE2	1:A:276:ALA:HB3	1.85	0.58
1:A:476:LEU:HD12	1:A:477:PHE:CE1	2.39	0.57
1:A:194:ARG:HH21	1:A:198:LEU:HD11	1.69	0.57
1:A:35:PRO:HD3	1:A:62:PRO:HA	1.85	0.57
1:A:241:VAL:HB	1:A:266:LEU:HD23	1.88	0.56
1:A:324:ILE:HD13	1:A:340:THR:HG22	1.86	0.56
1:A:12:TRP:CE2	1:A:131:VAL:HG22	2.41	0.55
1:A:431:LEU:HD22	1:A:459:VAL:HG22	1.88	0.55
1:A:193:ARG:H	1:A:193:ARG:HD2	1.71	0.55
1:A:59:LEU:CD2	1:A:74:LEU:HD23	2.38	0.54
1:A:278:GLY:HA2	1:A:281:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLY:HA3	1:A:457:VAL:HG13	1.90	0.54
1:A:35:PRO:HA	1:A:60:GLU:CD	2.33	0.53
1:A:63:ILE:CD1	1:A:95:VAL:HG11	2.38	0.53
1:A:298:CYS:SG	1:A:300:VAL:N	2.79	0.53
1:A:194:ARG:NH2	1:A:198:LEU:HD21	2.24	0.52
1:A:230:ALA:HA	1:A:449:ARG:HD2	1.91	0.52
1:A:154:GLU:O	1:A:155:LEU:HD23	2.09	0.52
1:A:130:ALA:HA	1:A:135:GLU:HG3	1.92	0.52
1:A:249:ALA:CB	1:A:417:MET:SD	2.98	0.51
1:A:282:LEU:HD22	1:A:286:LEU:HG	1.92	0.51
1:A:484:ARG:HA	1:A:487:LEU:HD12	1.92	0.51
1:A:283:ALA:O	1:A:287:ARG:HG3	2.10	0.50
1:A:324:ILE:HD11	1:A:341:VAL:HA	1.93	0.50
1:A:254:LEU:HD22	1:A:258:LEU:CD1	2.41	0.50
1:A:59:LEU:HD22	1:A:74:LEU:HD23	1.94	0.50
1:A:63:ILE:HG22	1:A:99:ASP:HB3	1.94	0.50
1:A:315:PRO:HD2	1:A:359:ILE:HD13	1.94	0.50
1:A:52:ARG:HD2	1:A:200:ALA:HB1	1.94	0.49
1:A:397:ARG:HE	1:A:404:ALA:HB2	1.78	0.49
1:A:414:GLY:O	2:A:593:HOH:O	2.19	0.48
1:A:75:LYS:HB3	1:A:76:PRO:HD3	1.95	0.48
1:A:287:ARG:HA	1:A:291:CYS:O	2.13	0.48
1:A:299:ASP:C	1:A:301:ALA:H	2.21	0.48
1:A:46:THR:HG22	1:A:56:VAL:CG1	2.39	0.47
1:A:254:LEU:HD22	1:A:258:LEU:HD11	1.95	0.47
1:A:214:VAL:HG22	1:A:219:ILE:HG22	1.97	0.47
1:A:229:ALA:O	1:A:449:ARG:HD2	2.15	0.47
1:A:75:LYS:HB3	1:A:76:PRO:CD	2.45	0.47
1:A:91:LEU:CD2	1:A:124:LEU:HD12	2.45	0.47
1:A:461:TRP:C	1:A:463:ARG:H	2.23	0.47
1:A:150:VAL:HG21	1:A:381:GLY:HA2	1.97	0.47
1:A:117:PRO:O	1:A:118:ALA:HB3	2.16	0.46
1:A:282:LEU:O	1:A:286:LEU:HG	2.16	0.45
1:A:270:SER:O	1:A:297:ALA:HA	2.16	0.45
1:A:419:ALA:HB1	1:A:423:GLU:HB2	1.98	0.45
1:A:426:LEU:HB3	1:A:431:LEU:HD12	1.98	0.45
1:A:224:VAL:HG22	1:A:476:LEU:O	2.17	0.45
1:A:194:ARG:CZ	1:A:198:LEU:HD21	2.47	0.45
1:A:126:ARG:CB	1:A:167:GLU:HG3	2.47	0.45
1:A:465:ALA:N	1:A:466:PRO:HD2	2.32	0.45
1:A:9:ARG:HH11	1:A:227:ALA:HB1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:CD2	1:A:163:ILE:HB	2.47	0.44
1:A:455:THR:CG2	1:A:457:VAL:HG23	2.45	0.44
1:A:338:PHE:CE1	1:A:342:ARG:HD2	2.53	0.44
1:A:333:LEU:CD1	2:A:550:HOH:O	2.66	0.44
1:A:431:LEU:CD2	1:A:459:VAL:HG22	2.48	0.44
1:A:50:SER:C	1:A:52:ARG:N	2.73	0.43
1:A:193:ARG:H	1:A:193:ARG:CD	2.32	0.43
1:A:461:TRP:CE2	1:A:480:VAL:HG11	2.53	0.43
1:A:37:THR:O	1:A:38:ASP:HB2	2.19	0.43
1:A:333:LEU:HD13	2:A:501:HOH:O	2.17	0.43
1:A:211:GLN:OE1	1:A:222:ARG:HD3	2.18	0.43
1:A:224:VAL:HG23	1:A:224:VAL:O	2.19	0.43
1:A:259:ALA:HA	1:A:263:ALA:HB3	2.01	0.43
1:A:66:ARG:HB2	1:A:69:GLU:OE2	2.19	0.42
1:A:333:LEU:HD11	1:A:382:ALA:HB2	2.01	0.42
1:A:398:ARG:HG3	1:A:452:VAL:HG22	2.02	0.42
1:A:482:GLU:H	1:A:482:GLU:CD	2.27	0.42
1:A:403:PRO:O	1:A:404:ALA:HB2	2.20	0.41
1:A:194:ARG:HA	1:A:197:GLU:HB2	2.02	0.41
1:A:47:THR:O	1:A:51:GLU:HG3	2.21	0.41
1:A:81:ALA:O	1:A:84:GLU:HB2	2.20	0.41
1:A:126:ARG:HD2	1:A:167:GLU:HG3	2.02	0.41
1:A:166:PRO:HG3	1:A:214:VAL:O	2.21	0.41
1:A:423:GLU:N	1:A:423:GLU:CD	2.79	0.41
1:A:476:LEU:HD12	1:A:477:PHE:CZ	2.56	0.40
1:A:91:LEU:HD21	1:A:124:LEU:HD12	2.03	0.40
1:A:126:ARG:O	1:A:126:ARG:HG3	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	447/511 (88%)	414 (93%)	29 (6%)	4 (1%)	14 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	ALA
1	A	38	ASP
1	A	300	VAL
1	A	35	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	321/373 (86%)	305 (95%)	16 (5%)	22 11

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	43	ASP
1	A	116	VAL
1	A	144	LEU
1	A	193	ARG
1	A	194	ARG
1	A	197	GLU
1	A	254	LEU
1	A	271	ARG
1	A	282	LEU
1	A	294	VAL
1	A	325	LEU
1	A	450	ASN
1	A	459	VAL
1	A	476	LEU
1	A	479	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	469	ASN

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	453/511 (88%)	1.23	102 (22%) 2 2	20, 40, 65, 82	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	THR	5.8
1	A	488	THR	5.0
1	A	300	VAL	4.6
1	A	487	LEU	4.5
1	A	298	CYS	4.4
1	A	204	ALA	4.4
1	A	362	LEU	4.3
1	A	15	LEU	4.2
1	A	166	PRO	4.1
1	A	118	ALA	4.1
1	A	216	ALA	4.1
1	A	477	PHE	4.0
1	A	54	ALA	3.9
1	A	476	LEU	3.9
1	A	27	GLY	3.7
1	A	53	GLY	3.6
1	A	224	VAL	3.6
1	A	220	TYR	3.6
1	A	214	VAL	3.3
1	A	36	THR	3.3
1	A	327	ASP	3.3
1	A	14	ALA	3.3
1	A	131	VAL	3.3
1	A	10	VAL	3.2
1	A	461	TRP	3.2
1	A	219	ILE	3.1
1	A	129	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	9	ARG	3.1
1	A	12	TRP	3.1
1	A	301	ALA	3.1
1	A	114	ILE	3.0
1	A	202	VAL	3.0
1	A	359	ILE	3.0
1	A	299	ASP	3.0
1	A	344	ALA	3.0
1	A	45	LEU	2.9
1	A	49	LEU	2.9
1	A	232	ALA	2.9
1	A	324	ILE	2.9
1	A	81	ALA	2.9
1	A	399	ALA	2.9
1	A	196	LEU	2.9
1	A	431	LEU	2.9
1	A	50	SER	2.8
1	A	116	VAL	2.8
1	A	11	THR	2.8
1	A	117	PRO	2.8
1	A	132	VAL	2.8
1	A	233	ALA	2.8
1	A	459	VAL	2.7
1	A	465	ALA	2.7
1	A	5	ALA	2.7
1	A	486	ALA	2.7
1	A	55	SER	2.7
1	A	48	VAL	2.6
1	A	464	PHE	2.6
1	A	229	ALA	2.6
1	A	273	GLY	2.6
1	A	2	PRO	2.5
1	A	462	GLU	2.5
1	A	467	ALA	2.5
1	A	412	TRP	2.5
1	A	452	VAL	2.5
1	A	485	GLU	2.5
1	A	29	CYS	2.5
1	A	44	GLY	2.5
1	A	203	LEU	2.5
1	A	221	GLY	2.5
1	A	480	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	165	LEU	2.4
1	A	361	GLY	2.4
1	A	47	THR	2.4
1	A	481	PRO	2.4
1	A	471	ILE	2.4
1	A	51	GLU	2.4
1	A	208	GLY	2.3
1	A	167	GLU	2.3
1	A	201	ALA	2.3
1	A	430	GLY	2.3
1	A	198	LEU	2.3
1	A	130	ALA	2.2
1	A	31	LEU	2.2
1	A	82	GLY	2.2
1	A	56	VAL	2.2
1	A	325	LEU	2.2
1	A	478	ASP	2.2
1	A	192	ASN	2.2
1	A	199	ALA	2.2
1	A	213	ALA	2.2
1	A	479	THR	2.1
1	A	231	GLY	2.1
1	A	463	ARG	2.1
1	A	413	GLY	2.1
1	A	195	ALA	2.1
1	A	193	ARG	2.1
1	A	360	LYS	2.1
1	A	483	ALA	2.1
1	A	271	ARG	2.0
1	A	484	ARG	2.0
1	A	218	GLY	2.0
1	A	474	GLY	2.0
1	A	428	ARG	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.