



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:58 am GMT

PDB ID : 5E3V  
Title : Truncated X-ray crystal structure of Adenylosuccinate Lyase from Salmonella typhimurium  
Authors : Banerjee, S.; Agrawal, M.J.; Murthy, M.R.N.  
Deposited on : 2015-10-04  
Resolution : 2.72 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](mailto: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.

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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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

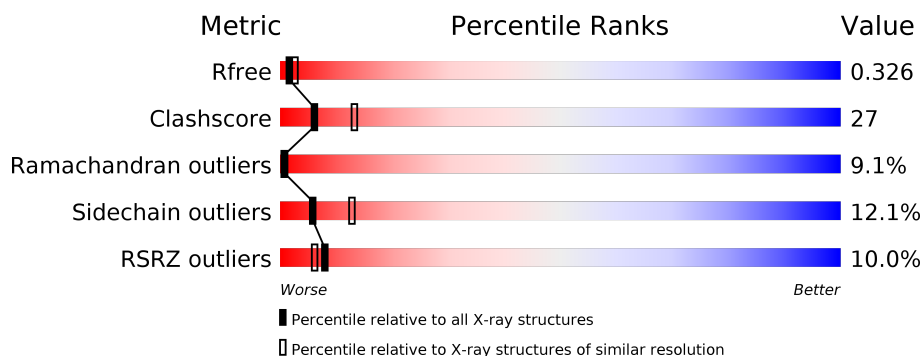
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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))
$R_{free}$	100719	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (2.74-2.70)

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  $\geq 3$ , 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	380	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2281 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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2262	1438	382	436	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A0F6B070
A	-12	ARG	-	expression tag	UNP A0A0F6B070
A	-11	GLY	-	expression tag	UNP A0A0F6B070
A	-10	SER	-	expression tag	UNP A0A0F6B070
A	-9	HIS	-	expression tag	UNP A0A0F6B070
A	-8	HIS	-	expression tag	UNP A0A0F6B070
A	-7	HIS	-	expression tag	UNP A0A0F6B070
A	-6	HIS	-	expression tag	UNP A0A0F6B070
A	-5	HIS	-	expression tag	UNP A0A0F6B070
A	-4	HIS	-	expression tag	UNP A0A0F6B070
A	-3	GLY	-	expression tag	UNP A0A0F6B070
A	-2	MET	-	expression tag	UNP A0A0F6B070
A	-1	ALA	-	expression tag	UNP A0A0F6B070
A	0	SER	-	expression tag	UNP A0A0F6B070

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.36Å 165.36Å 79.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.29 – 2.72 52.29 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (52.29-2.72) 99.8 (52.29-2.72)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.274 , 0.326 0.282 , 0.326	Depositor DCC
$R_{free}$ test set	760 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 113.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.82	0/2302	0.92	0/3139

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	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	TRP	Peptide
1	A	242	ASN	Peptide
1	A	243	PRO	Peptide
1	A	244	TYR	Peptide
1	A	252	ASP	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	2262	0	2020	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	0	3	0
All	All	2281	0	2020	117	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 27.

All (117) 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:245:THR:HG22	1:A:246:THR:H	1.06	1.13
1:A:243:PRO:HA	1:A:245:THR:O	1.50	1.12
1:A:248:ILE:O	1:A:250:PRO:HD3	1.52	1.09
1:A:227:HIS:O	1:A:228:GLN:HB2	1.55	0.99
1:A:167:LEU:HG	1:A:168:SER:H	1.30	0.94
1:A:245:THR:HG22	1:A:246:THR:N	1.87	0.87
1:A:46:LYS:HA	1:A:229:PHE:HZ	1.42	0.84
1:A:43:TRP:O	1:A:46:LYS:N	2.12	0.80
1:A:245:THR:CG2	1:A:246:THR:H	1.90	0.80
1:A:167:LEU:HG	1:A:168:SER:N	2.00	0.76
1:A:151:ILE:HG22	1:A:155:LYS:HE2	1.67	0.76
1:A:243:PRO:CA	1:A:245:THR:O	2.30	0.76
1:A:46:LYS:HA	1:A:229:PHE:CZ	2.22	0.73
1:A:166:LEU:N	1:A:166:LEU:HD12	2.08	0.69
1:A:80:ALA:O	1:A:84:THR:HG23	1.93	0.68
1:A:314:LEU:HG	1:A:356:ALA:CB	2.25	0.66
1:A:249:GLU:O	1:A:251:HIS:HB2	1.97	0.65
1:A:364:VAL:O	1:A:365:SER:CB	2.44	0.65
1:A:227:HIS:O	1:A:228:GLN:CB	2.33	0.65
1:A:251:HIS:O	1:A:252:ASP:OD2	2.15	0.65
1:A:161:TYR:HB3	1:A:180:LEU:O	1.97	0.63
1:A:363:GLY:O	1:A:364:VAL:HB	1.98	0.63
1:A:248:ILE:C	1:A:250:PRO:HD3	2.20	0.62
1:A:306:ASP:OD1	1:A:362:LYS:HE3	2.00	0.61
1:A:249:GLU:OE1	1:A:249:GLU:HA	2.00	0.61
1:A:30:TYR:HE1	1:A:75:ASN:C	2.05	0.60
1:A:229:PHE:O	1:A:229:PHE:HD1	1.85	0.60
1:A:39:VAL:HG12	1:A:126:ILE:HG23	1.84	0.59
1:A:243:PRO:C	1:A:245:THR:N	2.56	0.58
1:A:364:VAL:O	1:A:365:SER:OG	2.17	0.58
1:A:204:LEU:HD23	1:A:240:GLN:HB3	1.85	0.58
1:A:305:ILE:O	1:A:306:ASP:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:CG	1:A:355:ILE:HD12	2.39	0.57
1:A:32:LEU:HD12	1:A:33:LEU:N	2.21	0.56
1:A:16:TYR:CB	1:A:355:ILE:HD12	2.35	0.56
1:A:314:LEU:HG	1:A:356:ALA:HB1	1.88	0.56
1:A:139:ARG:HA	1:A:143:ILE:HD12	1.88	0.55
1:A:225:ASP:O	1:A:228:GLN:HB3	2.06	0.55
1:A:339:ASP:HB2	1:A:342:VAL:HB	1.87	0.55
1:A:161:TYR:HD2	1:A:184:MET:CE	2.20	0.55
1:A:198:LEU:O	1:A:199:ASN:CB	2.54	0.55
1:A:230:SER:O	1:A:234:VAL:HG23	2.07	0.54
1:A:306:ASP:CG	1:A:362:LYS:HE3	2.27	0.54
1:A:218:ILE:CB	2:A:416:HOH:O	2.55	0.53
1:A:306:ASP:OD1	1:A:362:LYS:CE	2.57	0.52
1:A:38:GLN:O	1:A:39:VAL:HB	2.09	0.52
1:A:344:ARG:NH1	2:A:402:HOH:O	2.43	0.52
1:A:197:GLN:C	1:A:198:LEU:O	2.43	0.51
1:A:360:THR:O	1:A:363:GLY:O	2.28	0.51
1:A:353:ALA:HB1	1:A:357:TYR:CZ	2.44	0.51
1:A:48:ALA:C	1:A:50:HIS:H	2.14	0.51
1:A:18:ASP:N	1:A:18:ASP:OD1	2.44	0.51
1:A:142:VAL:O	1:A:143:ILE:C	2.46	0.51
1:A:168:SER:HA	1:A:174:PRO:O	2.10	0.51
1:A:37:VAL:O	1:A:41:VAL:N	2.45	0.50
1:A:86:GLU:O	1:A:88:THR:HG23	2.11	0.50
1:A:363:GLY:O	1:A:364:VAL:CB	2.60	0.50
1:A:217:HIS:O	1:A:219:ALA:N	2.45	0.49
1:A:322:HIS:O	1:A:326:ASN:OD1	2.30	0.49
1:A:305:ILE:O	1:A:306:ASP:CB	2.60	0.49
1:A:242:ASN:HB3	1:A:243:PRO:CD	2.42	0.49
1:A:1:MET:O	1:A:2:GLU:O	2.29	0.49
1:A:104:VAL:O	1:A:104:VAL:HG13	2.13	0.49
1:A:43:TRP:O	1:A:46:LYS:CB	2.60	0.49
1:A:94:LYS:O	1:A:98:TYR:CE2	2.66	0.49
1:A:30:TYR:CE2	1:A:34:LYS:HD3	2.48	0.48
1:A:135:LEU:HD13	1:A:253:TYR:HE1	1.79	0.48
1:A:30:TYR:HE2	1:A:34:LYS:HD3	1.77	0.48
1:A:161:TYR:CD2	1:A:184:MET:HE1	2.48	0.48
1:A:201:VAL:HG11	1:A:257:LEU:HG	1.96	0.48
1:A:229:PHE:CD1	1:A:229:PHE:O	2.67	0.47
1:A:135:LEU:HD22	1:A:257:LEU:HD13	1.95	0.47
1:A:41:VAL:HA	1:A:44:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:CB	1:A:243:PRO:HD3	2.45	0.46
1:A:324:LEU:HD22	1:A:342:VAL:HG13	1.97	0.46
1:A:101:LYS:O	1:A:104:VAL:HB	2.15	0.46
1:A:161:TYR:HD2	1:A:184:MET:HE1	1.79	0.45
1:A:167:LEU:CG	1:A:168:SER:N	2.70	0.45
1:A:158:ALA:HB1	1:A:181:GLY:O	2.15	0.45
1:A:265:ASN:CB	1:A:318:ASN:HD21	2.29	0.45
1:A:339:ASP:O	1:A:343:LEU:HB2	2.16	0.45
1:A:228:GLN:O	1:A:232:GLU:HB2	2.17	0.45
1:A:241:TRP:CB	1:A:242:ASN:HD22	2.30	0.45
1:A:243:PRO:O	1:A:245:THR:N	2.46	0.45
1:A:244:TYR:HA	1:A:244:TYR:HD1	1.46	0.45
1:A:322:HIS:O	1:A:323:HIS:C	2.54	0.45
1:A:81:ARG:O	1:A:85:ILE:HB	2.17	0.44
1:A:93:VAL:O	1:A:94:LYS:CB	2.64	0.44
1:A:86:GLU:O	1:A:88:THR:N	2.51	0.44
1:A:168:SER:O	1:A:169:ARG:CB	2.66	0.44
1:A:18:ASP:HA	1:A:21:SER:HB3	1.99	0.44
1:A:44:LEU:C	1:A:46:LYS:N	2.69	0.43
1:A:316:LEU:O	1:A:317:SER:C	2.56	0.43
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.69	0.43
1:A:173:GLN:HA	1:A:174:PRO:HD3	1.73	0.43
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.85	0.42
1:A:227:HIS:C	1:A:227:HIS:ND1	2.72	0.42
1:A:317:SER:O	1:A:318:ASN:C	2.56	0.42
1:A:265:ASN:HB2	1:A:318:ASN:HD21	1.85	0.42
1:A:161:TYR:HD2	1:A:184:MET:HE2	1.85	0.41
1:A:340:SER:HB2	2:A:405:HOH:O	2.19	0.41
1:A:38:GLN:O	1:A:39:VAL:CB	2.67	0.41
1:A:264:PHE:C	1:A:264:PHE:CD2	2.94	0.41
1:A:1:MET:C	1:A:2:GLU:O	2.58	0.41
1:A:166:LEU:HD11	1:A:179:THR:CA	2.51	0.41
1:A:281:LEU:O	1:A:284:PHE:CD2	2.74	0.41
1:A:102:GLU:C	1:A:104:VAL:H	2.23	0.41
1:A:150:VAL:O	1:A:154:VAL:HG23	2.20	0.41
1:A:161:TYR:HA	1:A:164:ILE:HD13	2.03	0.41
1:A:245:THR:CG2	1:A:246:THR:N	2.59	0.41
1:A:253:TYR:HA	1:A:256:GLU:HG3	2.03	0.41
1:A:265:ASN:HD21	1:A:353:ALA:HB2	1.86	0.41
1:A:35:PHE:CE2	1:A:134:MET:HA	2.56	0.41
1:A:198:LEU:O	1:A:199:ASN:HB2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:CB	1:A:243:PRO:CD	2.99	0.40
1:A:18:ASP:C	1:A:20:VAL:H	2.25	0.40
1:A:86:GLU:C	1:A:88:THR:H	2.25	0.40

There are no symmetry-related clashes.

## 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	298/380 (78%)	227 (76%)	44 (15%)	27 (9%)	<b>1</b> <b>1</b>

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	87	ARG
1	A	119	PHE
1	A	124	GLU
1	A	169	ARG
1	A	174	PRO
1	A	228	GLN
1	A	242	ASN
1	A	244	TYR
1	A	365	SER
1	A	160	GLN
1	A	218	ILE
1	A	243	PRO
1	A	249	GLU
1	A	306	ASP
1	A	312	GLY
1	A	47	LEU
1	A	94	LYS

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Mol	Chain	Res	Type
1	A	168	SER
1	A	170	THR
1	A	167	LEU
1	A	247	GLN
1	A	177	PRO
1	A	364	VAL
1	A	39	VAL
1	A	275	VAL
1	A	142	VAL

### 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	206/320 (64%)	181 (88%)	25 (12%)	6 13

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

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	SER
1	A	12	VAL
1	A	18	ASP
1	A	41	VAL
1	A	78	ASP
1	A	85	ILE
1	A	90	ASN
1	A	92	ASP
1	A	104	VAL
1	A	125	ASP
1	A	130	SER
1	A	157	LEU
1	A	166	LEU
1	A	171	HIS
1	A	229	PHE
1	A	235	THR

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Mol	Chain	Res	Type
1	A	244	TYR
1	A	247	GLN
1	A	279	ILE
1	A	284	PHE
1	A	305	ILE
1	A	326	ASN
1	A	339	ASP
1	A	341	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	90	ASN
1	A	194	GLN
1	A	240	GLN
1	A	242	ASN
1	A	318	ASN
1	A	345	ASN
1	A	358	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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, 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	310/380 (81%)	0.53	31 (10%) 8 6	38, 81, 149, 195	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	ASN	5.9
1	A	170	THR	5.8
1	A	91	HIS	4.9
1	A	171	HIS	4.9
1	A	172	GLY	4.6
1	A	93	VAL	4.3
1	A	92	ASP	4.0
1	A	285	LYS	3.8
1	A	338	THR	3.5
1	A	89	THR	3.2
1	A	221	TYR	3.1
1	A	244	TYR	3.0
1	A	99	PHE	3.0
1	A	284	PHE	3.0
1	A	174	PRO	2.9
1	A	73	ASN	2.8
1	A	178	SER	2.8
1	A	217	HIS	2.7
1	A	177	PRO	2.7
1	A	71	VAL	2.6
1	A	44	LEU	2.6
1	A	50	HIS	2.4
1	A	157	LEU	2.4
1	A	100	LEU	2.4
1	A	104	VAL	2.4
1	A	220	ALA	2.3
1	A	96	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	168	SER	2.2
1	A	317	SER	2.2
1	A	163	ASP	2.1
1	A	219	ALA	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.