



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:50 am GMT

PDB ID : 3IPL  
Title : CRYSTAL STRUCTURE OF o-succinylbenzoic acid-CoA ligase FROM Staphylococcus aureus subsp. aureus Mu50  
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Deposited on : 2009-08-17  
Resolution : 2.30 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

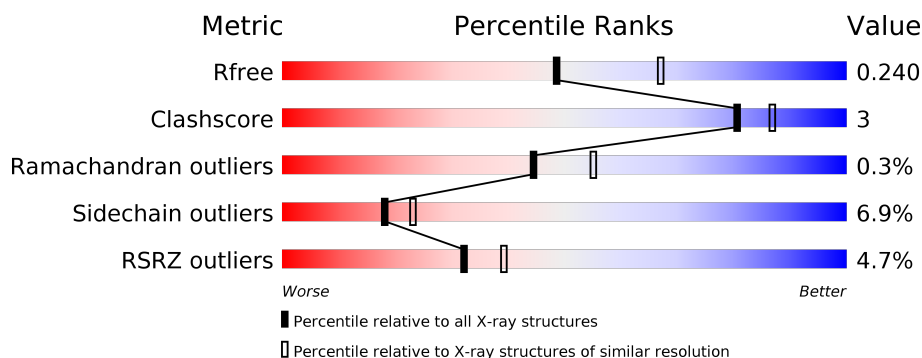
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	501	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	501	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	501	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>7%</div> <div>•</div> <div>29%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10478 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 2-succinylbenzoate--CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	11	0
			3588	2293	602	674	19			
1	B	445	Total	C	N	O	S	0	13	0
			3600	2303	600	676	21			
1	C	357	Total	C	N	O	S	0	10	0
			2873	1831	475	548	19			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P63526
A	1	LEU	-	EXPRESSION TAG	UNP P63526
A	492	GLU	-	EXPRESSION TAG	UNP P63526
A	493	GLY	-	EXPRESSION TAG	UNP P63526
A	494	HIS	-	EXPRESSION TAG	UNP P63526
A	495	HIS	-	EXPRESSION TAG	UNP P63526
A	496	HIS	-	EXPRESSION TAG	UNP P63526
A	497	HIS	-	EXPRESSION TAG	UNP P63526
A	498	HIS	-	EXPRESSION TAG	UNP P63526
A	499	HIS	-	EXPRESSION TAG	UNP P63526
B	0	SER	-	EXPRESSION TAG	UNP P63526
B	1	LEU	-	EXPRESSION TAG	UNP P63526
B	492	GLU	-	EXPRESSION TAG	UNP P63526
B	493	GLY	-	EXPRESSION TAG	UNP P63526
B	494	HIS	-	EXPRESSION TAG	UNP P63526
B	495	HIS	-	EXPRESSION TAG	UNP P63526
B	496	HIS	-	EXPRESSION TAG	UNP P63526
B	497	HIS	-	EXPRESSION TAG	UNP P63526
B	498	HIS	-	EXPRESSION TAG	UNP P63526
B	499	HIS	-	EXPRESSION TAG	UNP P63526
C	0	SER	-	EXPRESSION TAG	UNP P63526
C	1	LEU	-	EXPRESSION TAG	UNP P63526
C	492	GLU	-	EXPRESSION TAG	UNP P63526

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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLY	-	EXPRESSION TAG	UNP P63526
C	494	HIS	-	EXPRESSION TAG	UNP P63526
C	495	HIS	-	EXPRESSION TAG	UNP P63526
C	496	HIS	-	EXPRESSION TAG	UNP P63526
C	497	HIS	-	EXPRESSION TAG	UNP P63526
C	498	HIS	-	EXPRESSION TAG	UNP P63526
C	499	HIS	-	EXPRESSION TAG	UNP P63526

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	162	Total 162	O 162	0	0
2	B	152	Total 152	O 152	0	0
2	C	103	Total 103	O 103	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.51Å 65.42Å 114.96Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 31.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 99.2 (31.04-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.185 , 0.241 0.184 , 0.240	Depositor DCC
$R_{free}$ test set	1311 reflections (2.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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	0.46	0/3699	0.61	0/5020
1	B	0.46	0/3714	0.63	0/5038
1	C	0.45	0/2958	0.64	0/4015
All	All	0.46	0/10371	0.63	0/14073

There are no bond length outliers.

There are no bond angle outliers.

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	3588	0	3594	26	0
1	B	3600	0	3603	24	0
1	C	2873	0	2858	16	0
2	A	162	0	0	2	0
2	B	152	0	0	0	0
2	C	103	0	0	1	0
All	All	10478	0	10055	63	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 3.

All (63) 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:208:VAL:HG13	1:A:233:VAL:HG22	1.46	0.98
1:A:208:VAL:CG1	1:A:233:VAL:HG22	2.11	0.81
1:A:149:SER:HB2	1:A:152:ASN:HD22	1.58	0.67
1:B:242:LEU:HD22	1:B:246:LYS:HE3	1.75	0.67
1:A:208:VAL:HG13	1:A:233:VAL:CG2	2.23	0.65
1:C:383:ILE:HG12	1:C:389:VAL:HG22	1.84	0.59
1:C:180:PRO:HG3	1:C:361:LEU:HD13	1.86	0.56
1:B:383:ILE:HG12	1:B:389:VAL:HG22	1.88	0.56
1:A:206:LEU:HD23	1:A:208:VAL:HG22	1.87	0.55
1:A:180:PRO:HG3	1:A:361:LEU:HD13	1.88	0.55
1:A:19:THR:HG22	1:A:21:GLY:H	1.71	0.55
1:A:206:LEU:CD2	1:A:208:VAL:HG22	2.38	0.53
1:C:19:THR:HG23	1:C:231:ARG:HD3	1.89	0.53
1:A:246:LYS:NZ	2:A:515:HOH:O	2.43	0.51
1:B:167:MET:HE1	1:B:306:THR:HG23	1.91	0.51
1:B:418:PHE:HB3	1:B:421:ILE:HD12	1.92	0.51
1:C:77:ASN:HB3	1:C:80:LEU:HD22	1.93	0.51
1:B:338:ILE:HD13	1:B:383:ILE:HG13	1.93	0.50
1:B:450:LYS:HE3	1:B:470:PHE:HB2	1.92	0.50
1:B:185:ASN:HB3	1:B:309:CYS:SG	2.52	0.49
1:B:304:GLY:HA3	1:B:311:GLN:HA	1.95	0.48
1:B:113:LEU:HD12	1:B:116:ILE:HD12	1.96	0.48
1:A:58:GLN:NE2	2:A:577:HOH:O	2.48	0.47
1:A:90[B]:ARG:HH22	1:A:107:GLY:HA3	1.80	0.47
1:C:338:ILE:HD13	1:C:383:ILE:HG13	1.96	0.47
1:A:446:SER:HB2	1:A:447:ASP:H	1.59	0.47
1:B:348:GLU:HB2	1:B:350:MET:CE	2.45	0.47
1:B:336:VAL:HG12	1:B:383:ILE:HD11	1.98	0.46
1:A:383:ILE:HG12	1:A:389:VAL:HG22	1.98	0.46
1:A:185:ASN:HB3	1:A:309:CYS:SG	2.56	0.46
1:B:342:ASN:HB2	1:B:346:HIS:H	1.81	0.45
1:C:162:ASP:HB2	2:C:510:HOH:O	2.16	0.45
1:C:18:ILE:HG13	1:C:25:TYR:HB2	1.98	0.45
1:A:58:GLN:HB3	1:A:58:GLN:HE21	1.63	0.45
1:B:339:LYS:HB3	1:B:348:GLU:HG3	1.99	0.45
1:A:218:SER:HA	1:A:221:LEU:HD12	1.98	0.45
1:A:366:LEU:O	1:C:265:GLN:HG2	2.16	0.45
1:C:309:CYS:O	1:C:310[A]:SER:HB2	2.17	0.45
1:A:414:VAL:HG12	1:A:457:LEU:HD12	1.99	0.45
1:A:450:LYS:HE3	1:A:470:PHE:HB2	1.99	0.44
1:B:80:LEU:HG	1:B:84:GLU:HB3	1.99	0.44
1:A:370:PHE:HB2	1:C:266:GLN:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:MET:HE2	1:B:167:MET:HB3	1.85	0.43
1:C:304:GLY:HA3	1:C:311:GLN:HA	1.99	0.43
1:B:270:GLU:HG2	1:B:271:PRO:HD2	1.99	0.43
1:C:171:GLY:HA3	1:C:176:GLN:HG3	2.01	0.43
1:B:177[B]:LYS:HG2	1:B:363:PRO:HD2	2.00	0.43
1:B:351:ILE:HG12	1:B:352:LYS:N	2.34	0.42
1:C:89:MET:HB3	1:C:94:VAL:HG22	2.00	0.42
1:A:288:MET:HG3	1:B:364:THR:HG21	2.01	0.42
1:C:18:ILE:HG22	1:C:230:VAL:HG13	2.01	0.42
1:B:167:MET:CE	1:B:306:THR:HG23	2.50	0.42
1:A:22:GLN:HB2	1:A:22:GLN:HE21	1.67	0.41
1:A:336:VAL:HG13	1:A:349:LEU:HD11	2.02	0.41
1:C:177:LYS:HG3	1:C:363:PRO:HD3	2.02	0.41
1:B:149:SER:HA	1:B:150:PRO:HD3	1.96	0.41
1:A:57:ILE:O	1:A:61:ILE:HG12	2.20	0.40
1:A:100:THR:HG22	1:A:113:LEU:HD22	2.03	0.40
1:A:304:GLY:HA3	1:A:311[A]:GLN:HA	2.03	0.40
1:B:429:HIS:HB3	1:B:437:VAL:HG23	2.03	0.40
1:B:342:ASN:HB3	1:B:344[A]:GLU:H	1.87	0.40
1:C:57:ILE:O	1:C:61:ILE:HG12	2.21	0.40
1:B:342:ASN:HB3	1:B:344[B]:GLU:H	1.87	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	452/501 (90%)	437 (97%)	14 (3%)	1 (0%)	51	63
1	B	454/501 (91%)	441 (97%)	12 (3%)	1 (0%)	51	63
1	C	363/501 (72%)	351 (97%)	9 (2%)	3 (1%)	22	26
All	All	1269/1503 (84%)	1229 (97%)	35 (3%)	5 (0%)	44	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	SER
1	B	310	SER
1	C	310[A]	SER
1	C	310[B]	SER
1	C	102	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	401/440 (91%)	371 (92%)	30 (8%)	16	19
1	B	403/440 (92%)	372 (92%)	31 (8%)	15	18
1	C	322/440 (73%)	304 (94%)	18 (6%)	25	33
All	All	1126/1320 (85%)	1047 (93%)	79 (7%)	18	22

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	12	ASN
1	A	24	SER
1	A	58	GLN
1	A	59[A]	SER
1	A	59[B]	SER
1	A	80	LEU
1	A	94	VAL
1	A	95	GLN
1	A	101	LEU
1	A	148	GLU
1	A	154	LEU
1	A	208	VAL
1	A	233	VAL
1	A	290	GLU
1	A	329	MET

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Mol	Chain	Res	Type
1	A	337	LYS
1	A	339	LYS
1	A	343	LYS
1	A	351	ILE
1	A	361	LEU
1	A	369	THR
1	A	394[A]	ARG
1	A	394[B]	ARG
1	A	398	LEU
1	A	406	ILE
1	A	433	THR
1	A	446	SER
1	A	457	LEU
1	A	463	LYS
1	B	2[A]	ASP
1	B	2[B]	ASP
1	B	12	ASN
1	B	19	THR
1	B	40	ARG
1	B	42	LYS
1	B	79[A]	ARG
1	B	79[B]	ARG
1	B	80	LEU
1	B	89	MET
1	B	94	VAL
1	B	105	LEU
1	B	200	ASP
1	B	233	VAL
1	B	242	LEU
1	B	284	LEU
1	B	305	MET
1	B	311	GLN
1	B	331	SER
1	B	346	HIS
1	B	348	GLU
1	B	351	ILE
1	B	361	LEU
1	B	366	LEU
1	B	396	LYS
1	B	398	LEU
1	B	432	ASP
1	B	447	ASP

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Mol	Chain	Res	Type
1	B	457	LEU
1	B	463	LYS
1	B	474	ASP
1	C	30	LEU
1	C	32	CYS
1	C	80	LEU
1	C	92	ILE
1	C	94	VAL
1	C	114	ASP
1	C	154	LEU
1	C	173	THR
1	C	177	LYS
1	C	230	VAL
1	C	242	LEU
1	C	305	MET
1	C	311	GLN
1	C	327	VAL
1	C	339	LYS
1	C	346	HIS
1	C	351	ILE
1	C	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	22	GLN
1	A	58	GLN
1	A	109	GLN
1	A	152	ASN
1	A	240	GLN
1	A	266	GLN
1	A	296	ASN
1	A	340	ASN
1	B	311	GLN
1	B	417	GLN
1	C	45	GLN
1	C	240	GLN
1	C	261	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 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, 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	445/501 (88%)	0.08	17 (3%) 41 48	24, 44, 76, 105	0
1	B	445/501 (88%)	0.18	33 (7%) 15 21	21, 43, 101, 127	0
1	C	357/501 (71%)	0.01	8 (2%) 62 69	26, 43, 77, 105	0
All	All	1247/1503 (82%)	0.09	58 (4%) 32 39	21, 43, 88, 127	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	475	THR	9.2
1	B	118	PHE	8.0
1	C	173	THR	6.8
1	B	432	ASP	5.6
1	A	149	SER	5.4
1	B	174	GLY	5.3
1	B	474	ASP	5.3
1	A	115	ASP	4.9
1	B	443	VAL	4.6
1	B	433	THR	4.6
1	B	473	VAL	4.6
1	B	152	ASN	4.5
1	B	173	THR	4.4
1	B	441	TYR	4.3
1	A	151	SER	4.0
1	B	437	VAL	3.7
1	B	395	ARG	3.7
1	A	150	PRO	3.7
1	B	409	TYR	3.7
1	B	434	TRP	3.7
1	C	385	HIS	3.6
1	B	151	SER	3.5
1	B	422	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	149	SER	3.4
1	A	153	ILE	3.3
1	B	153	ILE	3.2
1	C	117	GLU	3.1
1	A	106	ARG	3.1
1	B	471	GLU	3.1
1	B	472	LYS	3.0
1	B	155	ASN	3.0
1	B	396	LYS	2.9
1	A	45	GLN	2.8
1	A	90[A]	ARG	2.8
1	C	174	GLY	2.7
1	C	155	ASN	2.7
1	B	407	TYR	2.7
1	A	344	GLU	2.7
1	B	344[A]	GLU	2.6
1	A	154	LEU	2.6
1	A	60	ILE	2.6
1	B	398	LEU	2.6
1	A	432	ASP	2.6
1	B	397	ASP	2.5
1	B	106	ARG	2.5
1	A	434	TRP	2.5
1	B	343	LYS	2.4
1	C	343	LYS	2.4
1	C	1	LEU	2.4
1	B	154	LEU	2.4
1	B	430	PRO	2.3
1	A	104	GLU	2.3
1	A	343	LYS	2.3
1	C	365	ASP	2.2
1	B	423	ASP	2.1
1	A	83	ASN	2.1
1	A	403	GLY	2.1
1	B	469	HIS	2.1

## 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 [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.