



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:23 PM UTC

PDB ID : 6HZQ / pdb_00006hzq
Title : Apo structure of TP domain from Escherichia coli Penicillin-Binding Protein 3
Authors : Bellini, D.; Koekemoer, L.; Newman, H.; Dowson, C.G.
Deposited on : 2018-10-23
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

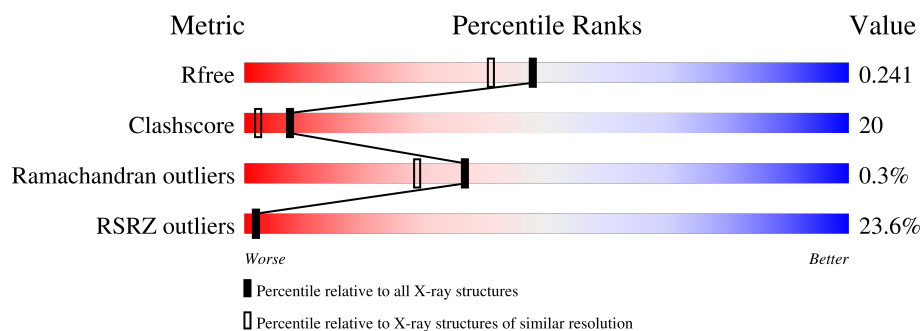
1 Overall quality at a glance

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))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	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	348	20% 58% 28% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2310 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 Peptidoglycan D,D-transpeptidase FtsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2259	1442	388	420	9			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	GLY	-	expression tag	UNP A0A0V7WLC6
A	228	PRO	-	expression tag	UNP A0A0V7WLC6
A	229	GLY	-	expression tag	UNP A0A0V7WLC6
A	230	TYR	-	expression tag	UNP A0A0V7WLC6
A	231	GLN	-	expression tag	UNP A0A0V7WLC6
A	232	ASP	-	expression tag	UNP A0A0V7WLC6
A	233	PRO	-	expression tag	UNP A0A0V7WLC6
A	?	-	SER	deletion	UNP A0A0V7WLC6
A	?	-	TYR	deletion	UNP A0A0V7WLC6
A	?	-	ASN	deletion	UNP A0A0V7WLC6
A	?	-	PRO	deletion	UNP A0A0V7WLC6
A	?	-	ASN	deletion	UNP A0A0V7WLC6
A	?	-	ASN	deletion	UNP A0A0V7WLC6
A	?	-	LEU	deletion	UNP A0A0V7WLC6
A	?	-	SER	deletion	UNP A0A0V7WLC6
A	?	-	GLY	deletion	UNP A0A0V7WLC6
A	?	-	THR	deletion	UNP A0A0V7WLC6
A	?	-	PRO	deletion	UNP A0A0V7WLC6
A	?	-	LYS	deletion	UNP A0A0V7WLC6
A	?	-	GLU	deletion	UNP A0A0V7WLC6
A	?	-	ALA	deletion	UNP A0A0V7WLC6
A	294	GLY	MET	conflict	UNP A0A0V7WLC6

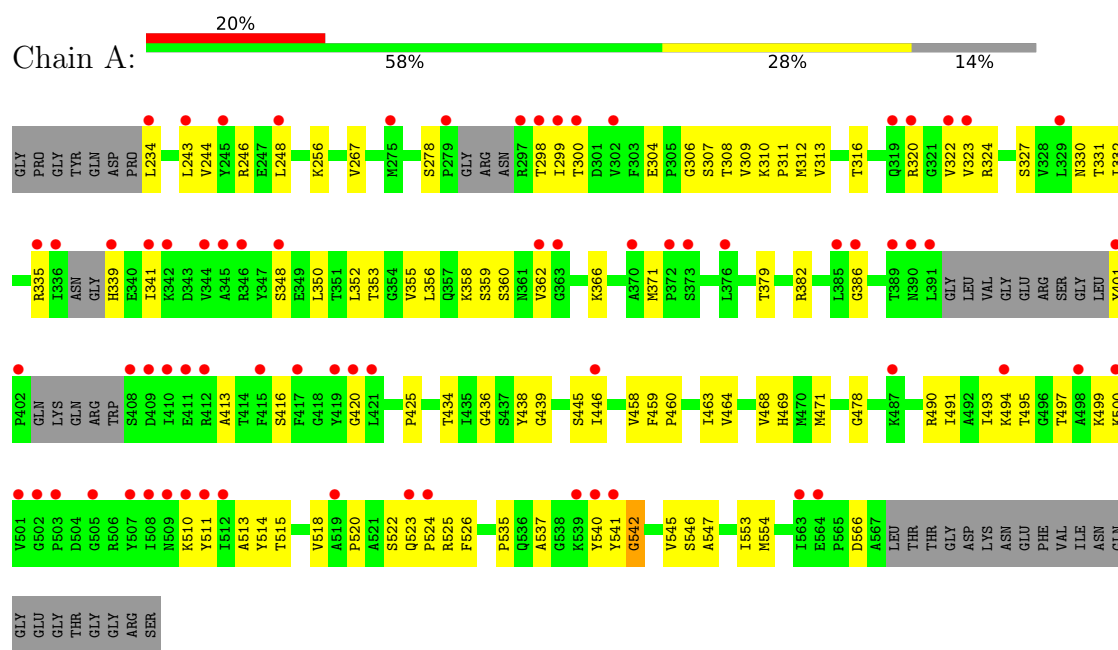
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		

3 Residue-property plots [i](#)

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: Peptidoglycan D,D-transpeptidase FtsI



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.87Å 150.03Å 43.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.35 – 1.95 78.35 – 1.95	Depositor EDS
% Data completeness (in resolution range)	53.6 (78.35-1.95) 53.6 (78.35-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.273 , 0.280 (Not available) , 0.241	Depositor DCC
R_{free} test set	549 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.001 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2310	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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	0.87	0/2298	1.21	6/3119 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	469	HIS	CA-C-N	5.20	127.51	120.38
1	A	469	HIS	C-N-CA	5.20	127.51	120.38
1	A	554	MET	CA-C-N	5.03	125.68	119.99
1	A	554	MET	C-N-CA	5.03	125.68	119.99
1	A	353	THR	CA-C-N	5.02	125.66	119.99
1	A	353	THR	C-N-CA	5.02	125.66	119.99

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	2259	0	2323	93	1
2	A	51	0	0	4	0
All	All	2310	0	2323	93	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 20.

All (93) 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:520:PRO:O	1:A:523:GLN:O	1.77	1.02
1:A:300:THR:HG23	1:A:425:PRO:HG2	1.46	0.95
1:A:495:THR:HG21	1:A:547:ALA:HB2	1.61	0.83
1:A:323:VAL:HG13	1:A:327:SER:HB2	1.61	0.81
1:A:300:THR:CG2	1:A:425:PRO:HD2	2.11	0.80
1:A:495:THR:HG22	1:A:515:THR:OG1	1.82	0.79
1:A:471:MET:HG2	1:A:494:LYS:HE2	1.64	0.79
1:A:310:LYS:NZ	1:A:359:SER:OG	2.16	0.79
1:A:323:VAL:HG13	1:A:327:SER:CB	2.13	0.78
1:A:323:VAL:HG11	1:A:352:LEU:HD11	1.67	0.77
1:A:323:VAL:CG1	1:A:327:SER:HB2	2.16	0.75
1:A:300:THR:HG22	1:A:425:PRO:HD2	1.69	0.74
1:A:300:THR:HG23	1:A:425:PRO:CG	2.17	0.74
1:A:356:LEU:HD22	1:A:494:LYS:HZ1	1.55	0.71
1:A:356:LEU:HB3	1:A:494:LYS:NZ	2.10	0.66
1:A:323:VAL:CG1	1:A:352:LEU:HD11	2.24	0.66
1:A:511:TYR:CE2	1:A:540:TYR:HD2	2.13	0.66
1:A:330:ASN:O	1:A:366:LYS:HE3	1.98	0.63
1:A:356:LEU:HD22	1:A:494:LYS:NZ	2.13	0.63
1:A:511:TYR:CE2	1:A:540:TYR:CD2	2.87	0.63
1:A:316:THR:HB	1:A:371:MET:HE1	1.80	0.63
1:A:316:THR:HG22	1:A:379:THR:OG1	1.99	0.62
1:A:497:THR:HG21	2:A:601:HOH:O	1.99	0.61
1:A:322:VAL:HG12	1:A:323:VAL:HG23	1.81	0.61
1:A:540:TYR:O	2:A:601:HOH:O	2.16	0.61
1:A:500:LYS:HB3	1:A:510:LYS:HB2	1.82	0.60
1:A:511:TYR:CZ	1:A:541:TYR:HB3	2.37	0.60
1:A:306:GLY:HA3	1:A:514:TYR:OH	2.01	0.59
1:A:459:PHE:CE1	1:A:463:ILE:HG21	2.39	0.58
1:A:520:PRO:O	1:A:523:GLN:C	2.46	0.58
1:A:511:TYR:CD2	1:A:540:TYR:HD2	2.22	0.57
1:A:499:LYS:HG2	1:A:511:TYR:CE1	2.41	0.56
1:A:522:SER:OG	1:A:566:ASP:OD1	2.15	0.56
1:A:300:THR:CG2	1:A:425:PRO:CD	2.84	0.55
1:A:459:PHE:HE1	1:A:463:ILE:HG21	1.72	0.55
1:A:497:THR:HG21	1:A:541:TYR:O	2.08	0.53
1:A:312:MET:O	1:A:316:THR:HG23	2.09	0.53
1:A:355:VAL:HG13	1:A:360:SER:HB3	1.91	0.53
1:A:446:ILE:N	2:A:602:HOH:O	2.25	0.52
1:A:518:VAL:HA	1:A:526:PHE:O	2.09	0.52
1:A:248:LEU:HG	1:A:278:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:NH2	1:A:458:VAL:O	2.43	0.51
1:A:267:VAL:CG1	1:A:436:GLY:C	2.84	0.51
1:A:313:VAL:O	1:A:316:THR:OG1	2.27	0.51
1:A:358:LYS:NZ	1:A:478:GLY:O	2.34	0.51
1:A:316:THR:CG2	1:A:379:THR:OG1	2.60	0.50
1:A:300:THR:CG2	1:A:425:PRO:CG	2.90	0.49
1:A:497:THR:HG22	1:A:513:ALA:HA	1.94	0.49
1:A:311:PRO:HD3	1:A:494:LYS:HE3	1.95	0.49
1:A:445:SER:HA	2:A:602:HOH:O	2.14	0.48
1:A:497:THR:HG21	1:A:542:GLY:O	2.14	0.48
1:A:434:THR:O	1:A:439:GLY:N	2.44	0.48
1:A:323:VAL:HG12	1:A:324:ARG:O	2.15	0.47
1:A:356:LEU:HB3	1:A:494:LYS:HZ1	1.79	0.47
1:A:332:ILE:HD13	1:A:348:SER:HA	1.96	0.47
1:A:320:ARG:HD3	1:A:371:MET:HG2	1.97	0.47
1:A:535:PRO:O	1:A:540:TYR:HB3	2.15	0.47
1:A:438:TYR:OH	1:A:524:PRO:HD2	2.15	0.46
1:A:335:ARG:HA	1:A:339:HIS:O	2.16	0.46
1:A:267:VAL:HG11	1:A:436:GLY:HA3	1.97	0.46
1:A:267:VAL:HG11	1:A:436:GLY:C	2.41	0.46
1:A:304:GLU:OE2	1:A:420:GLY:N	2.46	0.45
1:A:307:SER:N	1:A:514:TYR:OH	2.46	0.45
1:A:491:ILE:HD12	1:A:493:ILE:HG21	1.99	0.45
1:A:541:TYR:H	1:A:541:TYR:HD2	1.63	0.45
1:A:535:PRO:O	1:A:540:TYR:CB	2.64	0.45
1:A:234:LEU:CD2	1:A:446:ILE:HG13	2.47	0.45
1:A:541:TYR:O	1:A:542:GLY:C	2.60	0.45
1:A:300:THR:HG23	1:A:425:PRO:CD	2.47	0.45
1:A:513:ALA:CB	1:A:545:VAL:HB	2.47	0.45
1:A:464:VAL:O	1:A:468:VAL:HG23	2.17	0.45
1:A:331:THR:HG21	1:A:350:LEU:HD12	2.00	0.44
1:A:514:TYR:C	1:A:546:SER:OG	2.61	0.44
1:A:459:PHE:CD1	1:A:460:PRO:HD2	2.53	0.44
1:A:490:ARG:H	1:A:566:ASP:HB3	1.82	0.44
1:A:511:TYR:HE2	1:A:540:TYR:CD2	2.36	0.43
1:A:306:GLY:O	1:A:309:VAL:HG22	2.18	0.43
1:A:316:THR:CB	1:A:371:MET:HE1	2.46	0.43
1:A:520:PRO:HD2	1:A:523:GLN:O	2.19	0.43
1:A:413:ALA:O	1:A:416:SER:OG	2.31	0.43
1:A:497:THR:CG2	1:A:542:GLY:O	2.67	0.42
1:A:234:LEU:HD23	1:A:446:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HB3	1:A:246:ARG:NH2	2.35	0.42
1:A:298:THR:HG22	1:A:299:ILE:N	2.35	0.42
1:A:244:VAL:HG22	1:A:553:ILE:HG23	2.02	0.42
1:A:356:LEU:CD2	1:A:494:LYS:HZ1	2.26	0.42
1:A:308:THR:HG23	1:A:514:TYR:CE1	2.55	0.41
1:A:256:LYS:HD2	1:A:537:ALA:HB2	2.02	0.41
1:A:243:LEU:C	1:A:243:LEU:HD12	2.45	0.41
1:A:341:ILE:HG22	1:A:362:VAL:HG22	2.02	0.41
1:A:386:GLY:HA3	1:A:401:TYR:CD2	2.56	0.41
1:A:316:THR:HG23	1:A:379:THR:HG21	2.04	0.40
1:A:320:ARG:HH11	1:A:322:VAL:HG22	1.87	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:A:324:ARG:NH1	1:A:525:ARG:NH1[6_554]	2.09	0.11

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	291/348 (84%)	278 (96%)	12 (4%)	1 (0%)	36 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	301/348 (86%)	1.37	71 (23%) 2 2	2, 32, 79, 107	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	THR	7.0
1	A	503	PRO	6.7
1	A	401	TYR	6.4
1	A	507	TYR	6.2
1	A	410	ILE	5.8
1	A	508	ILE	5.4
1	A	541	TYR	5.1
1	A	502	GLY	5.1
1	A	509	ASN	5.1
1	A	540	TYR	4.9
1	A	336	ILE	4.9
1	A	501	VAL	4.9
1	A	511	TYR	4.8
1	A	523	GLN	4.5
1	A	299	ILE	4.3
1	A	539	LYS	4.1
1	A	510	LYS	4.1
1	A	279	PRO	4.0
1	A	419	TYR	3.8
1	A	420	GLY	3.7
1	A	421	LEU	3.6
1	A	339	HIS	3.6
1	A	409	ASP	3.6
1	A	412	ARG	3.5
1	A	323	VAL	3.4
1	A	341	ILE	3.4
1	A	415	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	390	ASN	3.4
1	A	494	LYS	3.3
1	A	302	VAL	3.3
1	A	346	ARG	3.3
1	A	329	LEU	3.2
1	A	402	PRO	3.2
1	A	344	VAL	3.2
1	A	505	GLY	3.2
1	A	298	THR	3.1
1	A	248	LEU	3.1
1	A	417	PHE	3.0
1	A	320	ARG	3.0
1	A	500	LYS	2.8
1	A	342	LYS	2.7
1	A	408	SER	2.7
1	A	370	ALA	2.7
1	A	245	TYR	2.6
1	A	391	LEU	2.6
1	A	372	PRO	2.6
1	A	376	LEU	2.6
1	A	487	LYS	2.5
1	A	363	GLY	2.5
1	A	297	ARG	2.5
1	A	345	ALA	2.4
1	A	524	PRO	2.4
1	A	319	GLN	2.4
1	A	385	LEU	2.4
1	A	335	ARG	2.4
1	A	373	SER	2.4
1	A	386	GLY	2.3
1	A	389	THR	2.3
1	A	512	ILE	2.2
1	A	498	ALA	2.2
1	A	519	ALA	2.2
1	A	563	ILE	2.2
1	A	362	VAL	2.2
1	A	411	GLU	2.2
1	A	322	VAL	2.2
1	A	446	ILE	2.1
1	A	348	SER	2.1
1	A	564	GLU	2.1
1	A	234	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	243	LEU	2.0
1	A	275	MET	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.