



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:07 PM UTC

PDB ID : 4G3U / pdb_00004g3u
Title : Mycobacterium smegmatis DprE1 - monoclinic crystal form
Authors : Li, H.; Jogl, G.
Deposited on : 2012-07-15
Resolution : 2.69 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

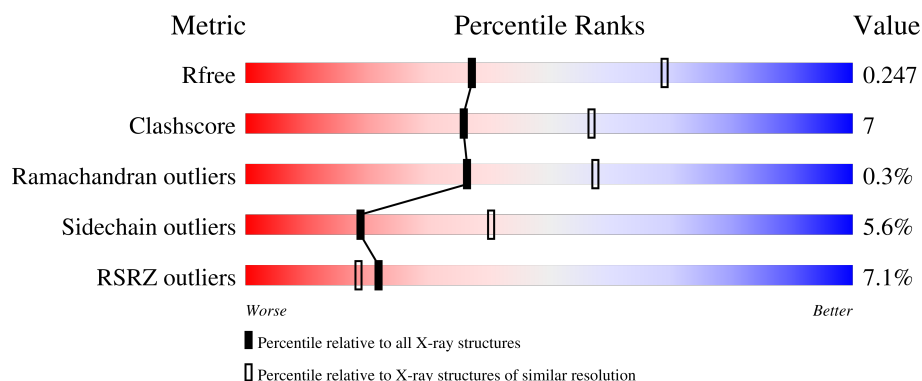
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	403	
1	B	403	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5657 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 oxidoreductase DprE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2685	1711	470	496	8			
1	B	346	Total	C	N	O	S	0	0	0
			2685	1711	470	496	8			

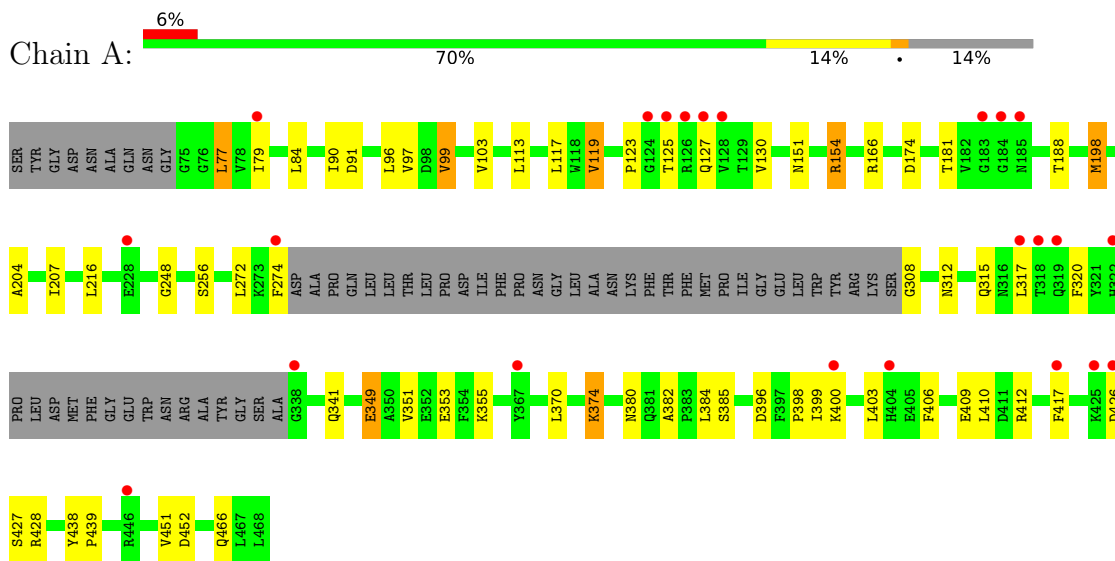
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	172	Total	O	0	0
			172	172		
2	B	115	Total	O	0	0
			115	115		

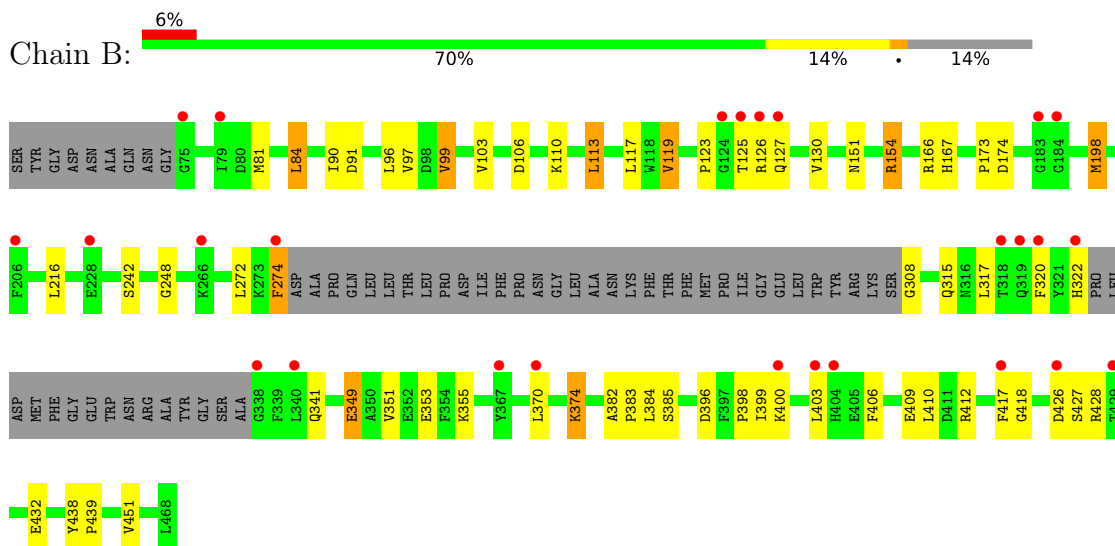
3 Residue-property plots [i](#)

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: oxidoreductase DprE1



- Molecule 1: oxidoreductase DprE1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.15Å 65.81Å 108.50Å 90.00° 109.00° 90.00°	Depositor
Resolution (Å)	34.20 – 2.69 34.20 – 2.69	Depositor EDS
% Data completeness (in resolution range)	92.8 (34.20-2.69) 92.8 (34.20-2.69)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX dev_1000	Depositor
R, R_{free}	0.220 , 0.254 0.217 , 0.247	Depositor DCC
R_{free} test set	1840 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5657	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	0.28	0/2751	0.73	2/3734 (0.1%)
1	B	0.29	0/2751	0.72	2/3734 (0.1%)
All	All	0.29	0/5502	0.72	4/7468 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	VAL	CA-C-N	5.47	125.12	119.05
1	B	119	VAL	C-N-CA	5.47	125.12	119.05
1	A	119	VAL	CA-C-N	5.36	125.00	119.05
1	A	119	VAL	C-N-CA	5.36	125.00	119.05

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	2685	0	2641	38	0
1	B	2685	0	2641	41	0
2	A	172	0	0	11	0
2	B	115	0	0	12	0
All	All	5657	0	5282	78	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 7.

All (78) 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:308:GLY:N	2:A:635:HOH:O	1.84	1.08
1:A:204:ALA:O	2:A:516:HOH:O	1.97	0.81
1:B:173:PRO:O	2:B:504:HOH:O	2.00	0.79
1:A:256:SER:OG	2:A:573:HOH:O	2.04	0.75
1:B:91:ASP:OD1	2:B:507:HOH:O	2.05	0.73
1:A:409:GLU:O	2:A:610:HOH:O	2.07	0.73
1:A:452:ASP:OD2	2:A:501:HOH:O	2.09	0.69
1:B:274:PHE:O	2:B:531:HOH:O	2.09	0.69
1:A:125:THR:HG22	1:A:127:GLN:H	1.57	0.69
1:B:125:THR:HG22	1:B:127:GLN:H	1.57	0.69
1:B:432:GLU:OE1	2:B:613:HOH:O	2.12	0.67
1:B:99:VAL:HG22	1:B:103:VAL:HG21	1.76	0.67
1:A:99:VAL:HG22	1:A:103:VAL:HG21	1.77	0.67
1:B:242:SER:OG	2:B:571:HOH:O	2.12	0.67
1:B:308:GLY:N	2:B:585:HOH:O	2.28	0.66
1:B:272:LEU:O	2:B:522:HOH:O	2.14	0.65
1:B:428:ARG:O	2:B:606:HOH:O	2.15	0.65
1:A:312:ASN:OD1	2:A:548:HOH:O	2.15	0.64
1:B:418:GLY:O	2:B:553:HOH:O	2.15	0.63
1:B:126:ARG:NH2	2:B:576:HOH:O	2.35	0.60
1:A:272:LEU:O	2:A:566:HOH:O	2.17	0.57
1:A:312:ASN:HA	2:A:548:HOH:O	2.07	0.54
1:A:427:SER:HA	1:A:428:ARG:HB3	1.88	0.54
1:B:427:SER:HA	1:B:428:ARG:HB3	1.89	0.54
1:A:166:ARG:NH2	1:A:174:ASP:OD1	2.38	0.52
1:A:398:PRO:HB2	1:A:400:LYS:HE2	1.93	0.50
1:A:341:GLN:NE2	1:A:396:ASP:OD2	2.45	0.50
1:B:398:PRO:HB2	1:B:400:LYS:HE2	1.94	0.50
1:B:341:GLN:NE2	1:B:396:ASP:OD2	2.45	0.50
1:A:91:ASP:OD1	1:B:167:HIS:NE2	2.41	0.49
1:A:315:GLN:HG3	1:A:320:PHE:HB2	1.95	0.48
1:A:353:GLU:OE1	1:A:353:GLU:N	2.43	0.48
1:A:399:ILE:HA	1:A:403:LEU:HD22	1.96	0.48
1:B:353:GLU:OE1	1:B:353:GLU:N	2.43	0.47
1:A:466:GLN:O	2:A:556:HOH:O	2.20	0.47
1:A:351:VAL:HG22	1:A:355:LYS:HE3	1.96	0.47
1:B:90:ILE:HG12	1:B:97:VAL:HG22	1.95	0.47
1:B:315:GLN:HG3	1:B:320:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASP:O	1:B:110:LYS:HG3	2.15	0.47
1:A:90:ILE:HG12	1:A:97:VAL:HG22	1.96	0.46
1:A:151:ASN:O	1:A:154:ARG:NH2	2.49	0.46
1:B:117:LEU:HB3	1:B:198:MET:HG2	1.97	0.46
1:B:151:ASN:ND2	2:B:551:HOH:O	2.48	0.46
1:B:322:HIS:ND1	2:B:581:HOH:O	2.16	0.46
1:B:351:VAL:HG22	1:B:355:LYS:HE3	1.97	0.46
1:A:117:LEU:HB3	1:A:198:MET:HG2	1.97	0.46
1:B:399:ILE:HA	1:B:403:LEU:HD22	1.99	0.45
1:A:166:ARG:NH1	2:A:588:HOH:O	2.34	0.45
1:B:382:ALA:HB3	1:B:385:SER:HB2	1.98	0.45
1:B:349:GLU:H	1:B:349:GLU:CD	2.25	0.45
1:A:349:GLU:H	1:A:349:GLU:CD	2.24	0.45
1:A:207:ILE:O	2:A:578:HOH:O	2.21	0.45
1:A:382:ALA:HB3	1:A:385:SER:HB2	1.98	0.45
1:B:166:ARG:NH2	1:B:174:ASP:OD1	2.38	0.45
1:A:151:ASN:CG	1:A:380:ASN:HD21	2.24	0.44
1:B:151:ASN:O	1:B:154:ARG:NH2	2.50	0.44
1:A:406:PHE:O	1:A:410:LEU:N	2.50	0.44
1:A:409:GLU:OE2	1:A:412:ARG:NH2	2.51	0.44
1:B:81:MET:HE3	1:B:84:LEU:HG	2.00	0.43
1:B:406:PHE:O	1:B:410:LEU:N	2.51	0.43
1:B:274:PHE:HD1	1:B:274:PHE:HA	1.73	0.43
1:B:216:LEU:HB2	1:B:248:GLY:HA3	2.00	0.43
1:B:99:VAL:HG11	1:B:130:VAL:HG21	2.00	0.43
1:B:409:GLU:OE2	1:B:412:ARG:NH2	2.51	0.43
1:A:438:TYR:HA	1:A:439:PRO:HD2	1.89	0.42
1:A:99:VAL:HG11	1:A:130:VAL:HG21	2.00	0.42
1:B:374:LYS:HB2	1:B:374:LYS:HE3	1.85	0.42
1:A:216:LEU:HB2	1:A:248:GLY:HA3	2.01	0.42
1:A:353:GLU:HB3	1:A:417:PHE:CD2	2.55	0.42
1:A:427:SER:HA	1:A:428:ARG:CB	2.50	0.42
1:B:353:GLU:HB3	1:B:417:PHE:CD2	2.55	0.42
1:B:382:ALA:HA	1:B:383:PRO:HD3	1.90	0.42
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.88	0.41
1:B:427:SER:HA	1:B:428:ARG:CB	2.50	0.41
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.86	0.41
1:A:374:LYS:HB2	1:A:374:LYS:HE3	1.86	0.41
1:B:438:TYR:HA	1:B:439:PRO:HD2	1.89	0.41
1:A:181:THR:HA	1:A:188:THR:HG21	2.04	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	340/403 (84%)	330 (97%)	9 (3%)	1 (0%)	36	57
1	B	340/403 (84%)	329 (97%)	10 (3%)	1 (0%)	36	57
All	All	680/806 (84%)	659 (97%)	19 (3%)	2 (0%)	36	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	PRO
1	B	123	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	286/332 (86%)	269 (94%)	17 (6%)	18	38
1	B	286/332 (86%)	271 (95%)	15 (5%)	21	43
All	All	572/664 (86%)	540 (94%)	32 (6%)	19	40

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	79	ILE
1	A	84	LEU
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	99	VAL
1	A	113	LEU
1	A	119	VAL
1	A	154	ARG
1	A	198	MET
1	A	274	PHE
1	A	317	LEU
1	A	349	GLU
1	A	370	LEU
1	A	374	LYS
1	A	384	LEU
1	A	426	ASP
1	A	451	VAL
1	B	84	LEU
1	B	96	LEU
1	B	99	VAL
1	B	113	LEU
1	B	119	VAL
1	B	154	ARG
1	B	198	MET
1	B	274	PHE
1	B	317	LEU
1	B	349	GLU
1	B	370	LEU
1	B	374	LYS
1	B	384	LEU
1	B	426	ASP
1	B	451	VAL

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

Mol	Chain	Res	Type
1	A	312	ASN
1	A	341	GLN
1	A	343	GLN
1	A	392	ASN
1	B	107	GLN
1	B	341	GLN
1	B	343	GLN
1	B	392	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	346/403 (85%)	0.32	23 (6%) 24 21	17, 40, 85, 115	0
1	B	346/403 (85%)	0.34	26 (7%) 20 17	17, 42, 85, 115	0
All	All	692/806 (85%)	0.33	49 (7%) 22 18	17, 41, 85, 115	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	HIS	5.1
1	B	322	HIS	5.0
1	A	319	GLN	4.8
1	A	274	PHE	4.8
1	A	426	ASP	4.6
1	A	228	GLU	3.5
1	A	126	ARG	3.5
1	B	79	ILE	3.4
1	A	318	THR	3.4
1	B	426	ASP	3.4
1	A	127	GLN	3.3
1	B	318	THR	3.2
1	A	404	HIS	3.1
1	B	228	GLU	3.1
1	A	400	LYS	3.1
1	B	338	GLY	3.0
1	A	367	TYR	2.9
1	B	400	LYS	2.9
1	A	417	PHE	2.9
1	A	124	GLY	2.8
1	B	404	HIS	2.8
1	B	75	GLY	2.8
1	B	183	GLY	2.8
1	A	184	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	125	THR	2.7
1	B	367	TYR	2.6
1	A	183	GLY	2.6
1	B	266	LYS	2.6
1	B	124	GLY	2.6
1	A	128	VAL	2.6
1	B	127	GLN	2.5
1	B	126	ARG	2.5
1	A	338	GLY	2.4
1	B	125	THR	2.4
1	B	274	PHE	2.4
1	A	317	LEU	2.4
1	B	184	GLY	2.3
1	B	340	LEU	2.3
1	A	425	LYS	2.2
1	B	417	PHE	2.2
1	B	320	PHE	2.2
1	A	185	ASN	2.2
1	B	403	LEU	2.2
1	A	79	ILE	2.2
1	B	206	PHE	2.2
1	B	429	THR	2.2
1	A	446	ARG	2.1
1	B	319	GLN	2.1
1	B	370	LEU	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.