Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 12:03 AM EDT

PDB ID	:	6N40
Title	:	Crystal structure of MmpL3 from Mycobacterium smegmatis
Authors	:	Su, C.-C.
Deposited on	:	2018-11-16
Resolution	:	3.31 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 (i) 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 (1)) were used in the production of this report:

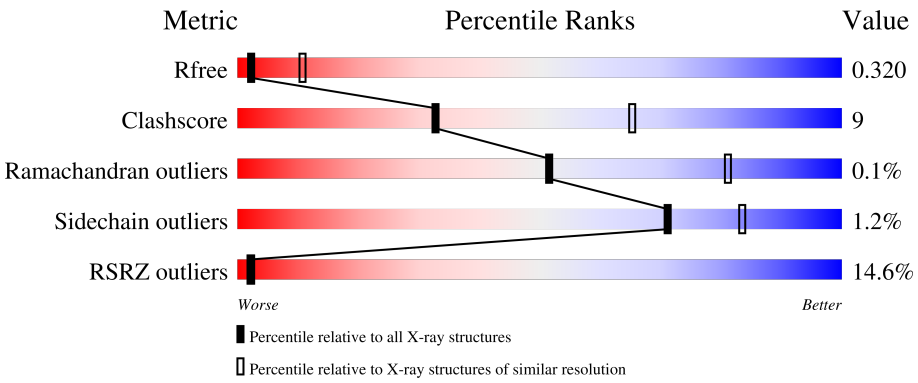
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	779	14% 74% 19% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5535 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 Membrane protein, MmpL family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	726	5535	3583	919	1005	28	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

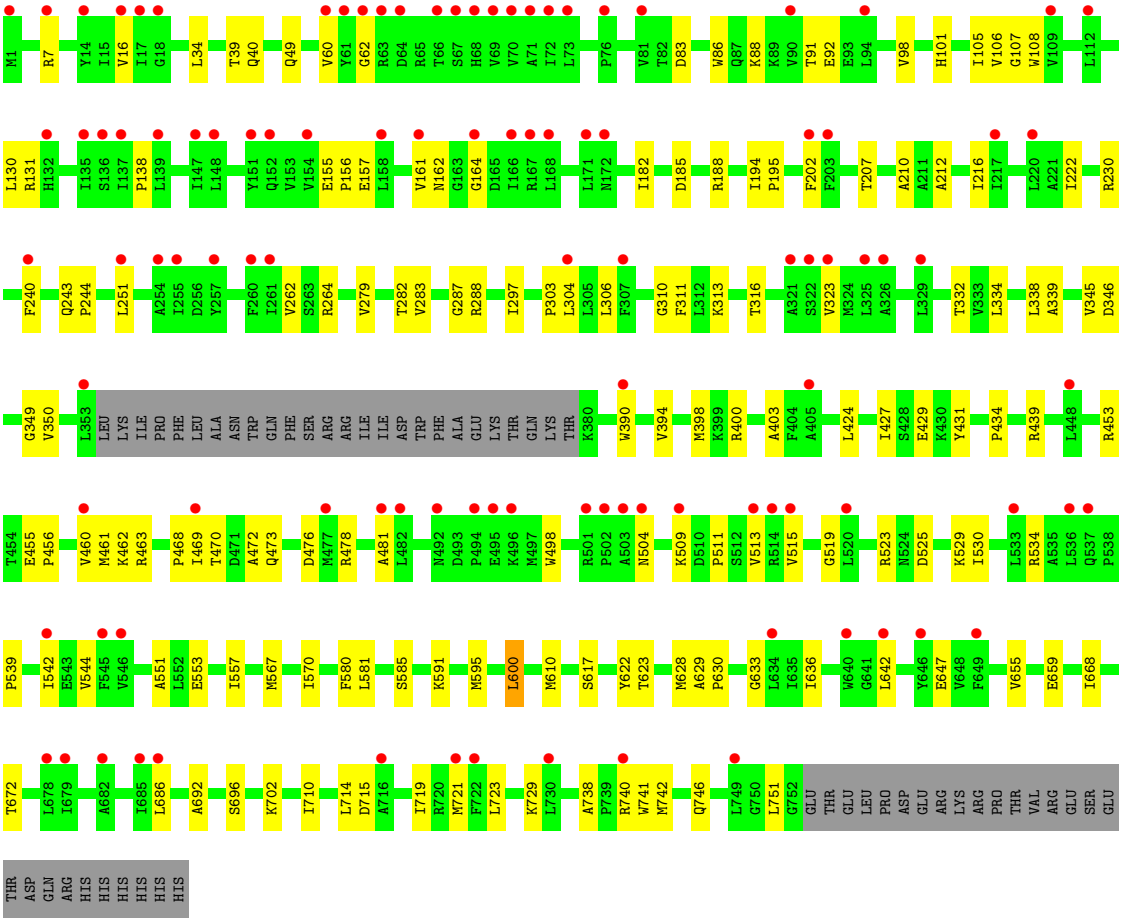
Chain	Residue	Modelled	Actual	Comment	Reference
A	774	HIS	-	expression tag	UNP A0QP27
A	775	HIS	-	expression tag	UNP A0QP27
A	776	HIS	-	expression tag	UNP A0QP27
A	777	HIS	-	expression tag	UNP A0QP27
A	778	HIS	-	expression tag	UNP A0QP27
A	779	HIS	-	expression tag	UNP A0QP27

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: Membrane protein, MmpL family protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.24Å 130.92Å 155.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.19 – 3.31 100.19 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.9 (100.19-3.31) 99.3 (100.19-3.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.14rc1_3177: ???)	Depositor
R, R_{free}	0.266 , 0.315 0.275 , 0.320	Depositor DCC
R_{free} test set	1306 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	118.3	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 65.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.27	0/5645	0.44	0/7681

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	5535	0	5705	98	0
All	All	5535	0	5705	98	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 9.

All (98) 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:696:SER:O	1:A:702:LYS:HE3	1.68	0.94
1:A:105:ILE:HG22	1:A:107:GLY:H	1.51	0.75
1:A:264:ARG:HG3	1:A:282:THR:HG22	1.75	0.69
1:A:628:MET:HG2	1:A:630:PRO:HD2	1.75	0.68
1:A:62:GLY:HA3	1:A:504:ASN:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:GLN:NE2	1:A:751:LEU:O	2.27	0.67
1:A:455:GLU:OE1	1:A:523:ARG:NH1	2.29	0.66
1:A:617:SER:HA	1:A:622:TYR:CE2	2.32	0.64
1:A:523:ARG:NH2	1:A:553:GLU:OE1	2.33	0.61
1:A:283:VAL:HA	1:A:287:GLY:HA3	1.81	0.60
1:A:262:VAL:HG23	1:A:334:LEU:HD21	1.82	0.60
1:A:429:GLU:OE2	1:A:453:ARG:NH1	2.35	0.60
1:A:222:ILE:HD11	1:A:251:LEU:HB2	1.83	0.59
1:A:207:THR:HG21	1:A:346:ASP:HA	1.85	0.58
1:A:434:PRO:HG3	1:A:623:THR:OG1	2.04	0.58
1:A:182:ILE:HG23	1:A:244:PRO:HG3	1.86	0.58
1:A:525:ASP:HB3	1:A:529:LYS:HD3	1.86	0.57
1:A:539:PRO:HD2	1:A:542:ILE:HD11	1.88	0.55
1:A:194:ILE:HG22	1:A:195:PRO:HD3	1.88	0.55
1:A:461:MET:HB2	1:A:542:ILE:HD12	1.87	0.55
1:A:210:ALA:HB2	1:A:345:VAL:HG12	1.88	0.55
1:A:83:ASP:OD1	1:A:86:TRP:N	2.35	0.54
1:A:303:PRO:HB2	1:A:567:MET:HG3	1.90	0.54
1:A:463:ARG:HD3	1:A:469:ILE:HG12	1.88	0.54
1:A:310:GLY:HA2	1:A:313:LYS:HE3	1.91	0.53
1:A:460:VAL:HA	1:A:515:VAL:HG12	1.91	0.52
1:A:580:PHE:CZ	1:A:742:MET:HB3	2.45	0.52
1:A:297:ILE:HG21	1:A:323:VAL:HG21	1.92	0.51
1:A:60:VAL:HG21	1:A:513:VAL:HB	1.93	0.51
1:A:306:LEU:HD11	1:A:570:ILE:HD12	1.93	0.50
1:A:60:VAL:HG13	1:A:509:LYS:HA	1.94	0.50
1:A:642:LEU:HD11	1:A:686:LEU:HD21	1.93	0.50
1:A:91:THR:HG23	1:A:108:TRP:HZ2	1.77	0.49
1:A:462:LYS:HB2	1:A:513:VAL:HG22	1.94	0.49
1:A:668:ILE:O	1:A:672:THR:HG22	2.13	0.49
1:A:207:THR:HG23	1:A:349:GLY:H	1.77	0.49
1:A:591:LYS:NZ	1:A:647:GLU:OE1	2.45	0.49
1:A:304:LEU:HB2	1:A:316:THR:HG21	1.95	0.49
1:A:161:VAL:HG23	1:A:162:ASN:H	1.76	0.49
1:A:202:PHE:HE1	1:A:350:VAL:HG22	1.77	0.49
1:A:394:VAL:HG21	1:A:672:THR:HG21	1.95	0.49
1:A:655:VAL:O	1:A:659:GLU:HG2	2.13	0.48
1:A:463:ARG:HH11	1:A:469:ILE:HA	1.79	0.48
1:A:262:VAL:HA	1:A:338:LEU:HD11	1.95	0.48
1:A:472:ALA:O	1:A:476:ASP:N	2.47	0.48
1:A:390:TRP:HZ3	1:A:721:MET:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ASP:HA	1:A:719:ILE:HB	1.96	0.47
1:A:49:GLN:HB3	1:A:534:ARG:HH12	1.80	0.47
1:A:530:ILE:HD13	1:A:551:ALA:HA	1.97	0.47
1:A:91:THR:HG23	1:A:108:TRP:CZ2	2.50	0.46
1:A:182:ILE:HD12	1:A:244:PRO:HG2	1.97	0.46
1:A:107:GLY:O	1:A:138:PRO:HD2	2.15	0.46
1:A:557:ILE:HG12	1:A:629:ALA:HB2	1.97	0.46
1:A:424:LEU:HD12	1:A:557:ILE:HG23	1.97	0.46
1:A:585:SER:HA	1:A:738:ALA:HB2	1.97	0.46
1:A:202:PHE:CE1	1:A:350:VAL:HG22	2.51	0.46
1:A:595:MET:HG2	1:A:719:ILE:HD12	1.99	0.45
1:A:88:LYS:O	1:A:92:GLU:HB2	2.17	0.45
1:A:478:ARG:HG3	1:A:498:TRP:HB2	2.00	0.44
1:A:394:VAL:HG21	1:A:672:THR:CG2	2.47	0.44
1:A:461:MET:HB3	1:A:544:VAL:HG22	1.99	0.44
1:A:101:HIS:NE2	1:A:157:GLU:OE1	2.41	0.44
1:A:212:ALA:O	1:A:216:ILE:HG12	2.18	0.44
1:A:98:VAL:HG11	1:A:107:GLY:HA2	2.00	0.44
1:A:696:SER:O	1:A:702:LYS:CE	2.55	0.43
1:A:39:THR:OG1	1:A:40:GLN:N	2.50	0.43
1:A:279:VAL:HG21	1:A:339:ALA:HB2	2.00	0.43
1:A:439:ARG:HH12	1:A:623:THR:HG21	1.83	0.43
1:A:463:ARG:NH1	1:A:473:GLN:OE1	2.52	0.42
1:A:473:GLN:HA	1:A:476:ASP:HB3	2.02	0.42
1:A:98:VAL:HG21	1:A:108:TRP:HD1	1.84	0.42
1:A:600:LEU:HD11	1:A:636:ILE:HG23	2.01	0.42
1:A:468:PRO:HA	1:A:511:PRO:O	2.19	0.41
1:A:427:ILE:HD12	1:A:431:TYR:CE2	2.55	0.41
1:A:106:VAL:CG2	1:A:138:PRO:HB2	2.50	0.41
1:A:155:GLU:N	1:A:156:PRO:HD2	2.35	0.41
1:A:185:ASP:OD2	1:A:696:SER:OG	2.38	0.41
1:A:710:ILE:O	1:A:714:LEU:HB2	2.20	0.41
1:A:130:LEU:O	1:A:131:ARG:HB2	2.20	0.41
1:A:243:GLN:HB2	1:A:244:PRO:HD3	2.01	0.41
1:A:288:ARG:NH2	1:A:581:LEU:O	2.54	0.41
1:A:481:ALA:HB1	1:A:498:TRP:CE2	2.55	0.41
1:A:400:ARG:HG3	1:A:403:ALA:HB3	2.01	0.41
1:A:264:ARG:HA	1:A:264:ARG:HD3	1.96	0.41
1:A:390:TRP:CZ3	1:A:721:MET:HG2	2.55	0.41
1:A:463:ARG:CG	1:A:542:ILE:HG22	2.50	0.41
1:A:207:THR:CG2	1:A:349:GLY:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:HD2	1:A:692:ALA:O	2.21	0.40
1:A:16:VAL:HG13	1:A:332:THR:HG23	2.03	0.40
1:A:456:PRO:HA	1:A:519:GLY:HA2	2.03	0.40
1:A:610:MET:O	1:A:622:TYR:OH	2.35	0.40
1:A:34:LEU:HD13	1:A:230:ARG:HA	2.04	0.40
1:A:470:THR:HB	1:A:473:GLN:HG3	2.02	0.40
1:A:304:LEU:HD21	1:A:633:GLY:O	2.22	0.40
1:A:530:ILE:HG22	1:A:534:ARG:HE	1.86	0.40
1:A:591:LYS:HE3	1:A:591:LYS:HB3	1.92	0.40
1:A:398:MET:HG2	1:A:729:LYS:HB2	2.03	0.40
1:A:617:SER:HA	1:A:622:TYR:CZ	2.56	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	722/779 (93%)	684 (95%)	37 (5%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	GLY

5.3.2 Protein sidechains (i)

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	590/643 (92%)	583 (99%)	7 (1%)	71 83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	240	PHE
1	A	311	PHE
1	A	600	LEU
1	A	723	LEU
1	A	740	ARG
1	A	741	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	726/779 (93%)	0.91	106 (14%) 2 2	93, 122, 160, 190	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	685	ILE	5.1
1	A	686	LEU	5.1
1	A	71	ALA	4.6
1	A	504	ASN	4.5
1	A	60	VAL	4.4
1	A	67	SER	4.4
1	A	546	VAL	4.4
1	A	171	LEU	4.2
1	A	61	TYR	4.2
1	A	73	LEU	4.2
1	A	307	PHE	4.1
1	A	147	ILE	4.0
1	A	537	GLN	4.0
1	A	492	ASN	3.9
1	A	502	PRO	3.8
1	A	304	LEU	3.8
1	A	496	LYS	3.8
1	A	69	VAL	3.8
1	A	740	ARG	3.8
1	A	254	ALA	3.8
1	A	642	LEU	3.7
1	A	172	ASN	3.7
1	A	168	LEU	3.7
1	A	203	PHE	3.6
1	A	7	ARG	3.4
1	A	353	LEU	3.4
1	A	81	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	72	ILE	3.4
1	A	148	LEU	3.3
1	A	482	LEU	3.3
1	A	76	PRO	3.2
1	A	716	ALA	3.2
1	A	139	LEU	3.2
1	A	136	SER	3.2
1	A	66	THR	3.2
1	A	257	TYR	3.1
1	A	514	ARG	3.1
1	A	682	ALA	3.1
1	A	501	ARG	3.0
1	A	14	TYR	2.9
1	A	164	GLY	2.9
1	A	390	TRP	2.9
1	A	721	MET	2.8
1	A	323	VAL	2.8
1	A	68	HIS	2.8
1	A	405	ALA	2.8
1	A	112	LEU	2.8
1	A	152	GLN	2.7
1	A	161	VAL	2.7
1	A	495	GLU	2.7
1	A	494	PRO	2.7
1	A	448	LEU	2.7
1	A	151	TYR	2.6
1	A	649	PHE	2.6
1	A	646	TYR	2.6
1	A	158	LEU	2.6
1	A	326	ALA	2.6
1	A	255	ILE	2.6
1	A	321	ALA	2.5
1	A	166	ILE	2.5
1	A	167	ARG	2.5
1	A	1	MET	2.5
1	A	749	LEU	2.5
1	A	132	HIS	2.5
1	A	261	ILE	2.5
1	A	18	GLY	2.5
1	A	542	ILE	2.4
1	A	513	VAL	2.4
1	A	678	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	2.4
1	A	137	ILE	2.4
1	A	90	VAL	2.4
1	A	520	LEU	2.4
1	A	251	LEU	2.4
1	A	94	LEU	2.3
1	A	503	ALA	2.3
1	A	62	GLY	2.3
1	A	679	ILE	2.3
1	A	154	VAL	2.3
1	A	640	TRP	2.3
1	A	17	ILE	2.3
1	A	515	VAL	2.2
1	A	533	LEU	2.2
1	A	481	ALA	2.2
1	A	240	PHE	2.2
1	A	460	VAL	2.2
1	A	135	ILE	2.2
1	A	260	PHE	2.2
1	A	469	ILE	2.2
1	A	202	PHE	2.2
1	A	217	ILE	2.2
1	A	63	ARG	2.2
1	A	509	LYS	2.2
1	A	536	LEU	2.2
1	A	477	MET	2.1
1	A	329	LEU	2.1
1	A	325	LEU	2.1
1	A	64	ASP	2.1
1	A	545	PHE	2.1
1	A	322	SER	2.1
1	A	634	LEU	2.1
1	A	730	LEU	2.1
1	A	722	PHE	2.0
1	A	220	LEU	2.0
1	A	16	VAL	2.0
1	A	109	VAL	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 monosaccharides 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.