



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:07 am GMT

PDB ID : 4J18  
Title : Crystal structure of H191L mutant of UDP-glucose pyrophosphorylase from Leishmania major  
Authors : Fuehring, J.I.; Routier, F.H.; Lamerz, A.-C.; Baruch, P.; Gerardy-Schahn, R.; Fedorov, R.  
Deposited on : 2013-02-01  
Resolution : 2.35 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

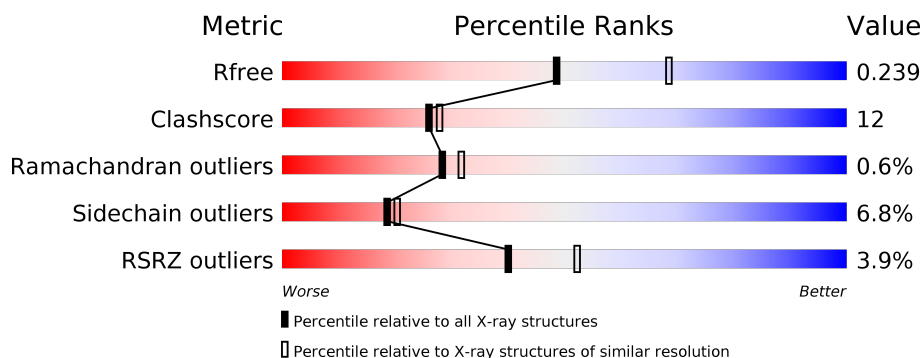
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	505	<div> <div>4%</div> <div>76%</div> <div>17%</div> <div>...</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4053 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 UDP-glucose pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	3744	2360	636	721	27	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	LEU	HIS	ENGINEERED MUTATION	UNP Q4QDU3
A	495	MET	-	EXPRESSION TAG	UNP Q4QDU3
A	496	ARG	-	EXPRESSION TAG	UNP Q4QDU3
A	497	PRO	-	EXPRESSION TAG	UNP Q4QDU3
A	498	LEU	-	EXPRESSION TAG	UNP Q4QDU3
A	499	GLU	-	EXPRESSION TAG	UNP Q4QDU3
A	500	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	501	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	502	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	503	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	504	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	505	HIS	-	EXPRESSION TAG	UNP Q4QDU3

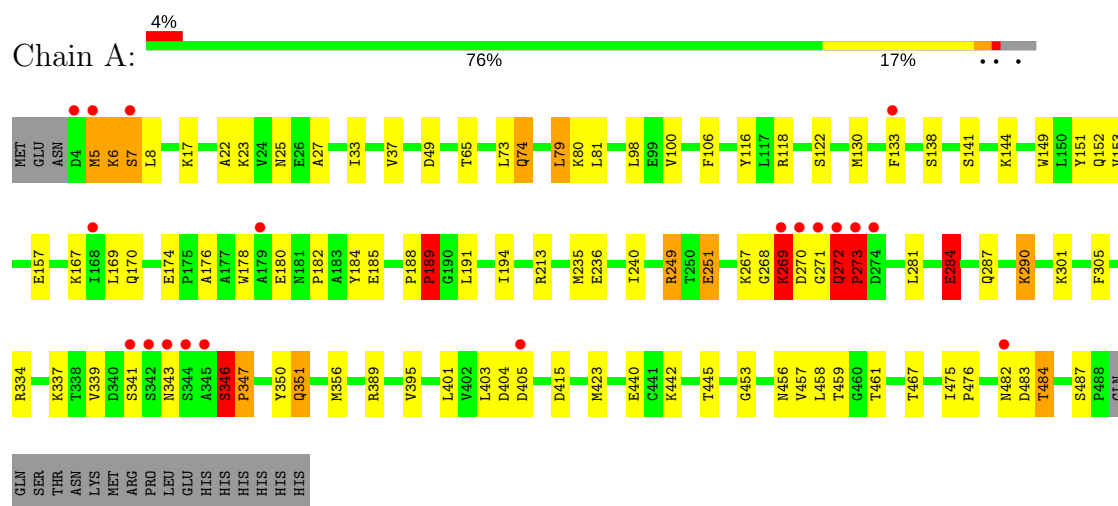
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	309	Total	O	0	0
			309	309		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: UDP-glucose pyrophosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.31Å 101.31Å 71.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.50 – 2.35 19.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.50-2.35) 99.4 (19.50-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.178 , 0.232 0.193 , 0.239	Depositor DCC
$R_{free}$ test set	1511 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4053	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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

### 5.1 Standard geometry

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	1.47	1/3813 (0.0%)	0.89	13/5164 (0.3%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	PRO	N-CD	5.05	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	487	SER	C-N-CD	6.54	142.13	128.40
1	A	272	GLN	C-N-CD	6.46	141.96	128.40
1	A	284	GLU	CB-CA-C	-6.03	98.35	110.40
1	A	269	LYS	CB-CA-C	-5.88	98.64	110.40
1	A	346	SER	C-N-CD	5.59	140.15	128.40
1	A	189	PRO	CA-C-N	5.59	127.37	116.20
1	A	7	SER	CB-CA-C	-5.46	99.72	110.10
1	A	273	PRO	CA-N-CD	-5.44	103.88	111.50
1	A	249	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	7	SER	N-CA-C	5.06	124.66	111.00
1	A	423	MET	CA-CB-CG	-5.05	104.71	113.30
1	A	189	PRO	N-CA-C	5.04	125.20	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	PRO	Peptide
1	A	22	ALA	Peptide

## 5.2 Too-close contacts

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	3744	0	3737	88	0
2	A	309	0	0	21	0
All	All	4053	0	3737	88	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 12.

All (88) 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:268:GLY:HA2	1:A:269:LYS:CB	1.53	1.35
1:A:268:GLY:CA	1:A:269:LYS:HB2	1.62	1.30
1:A:249:ARG:HG2	1:A:305:PHE:HB2	1.33	1.03
1:A:351:GLN:HB3	2:A:1279:HOH:O	1.59	1.00
1:A:339:VAL:HG12	1:A:346:SER:HB2	1.59	0.84
1:A:268:GLY:HA2	1:A:269:LYS:HB2	0.83	0.83
1:A:271:GLY:C	1:A:273:PRO:HD3	2.00	0.82
1:A:5:MET:O	1:A:7:SER:HB3	1.80	0.80
1:A:268:GLY:CA	1:A:269:LYS:CB	2.40	0.78
1:A:152:GLN:HG2	2:A:1266:HOH:O	1.84	0.77
1:A:284:GLU:H	1:A:287:GLN:HE21	1.32	0.77
1:A:267:LYS:O	1:A:269:LYS:HB2	1.85	0.76
1:A:167:LYS:HE3	1:A:184:TYR:O	1.86	0.76
1:A:133:PHE:CE2	2:A:1092:HOH:O	2.41	0.73
1:A:267:LYS:O	1:A:269:LYS:HG3	1.88	0.73
1:A:249:ARG:CG	1:A:305:PHE:HB2	2.15	0.73
1:A:149:TRP:HB2	2:A:1108:HOH:O	1.91	0.70
1:A:144:LYS:HB2	1:A:151:TYR:CD1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:HA	1:A:8:LEU:N	2.09	0.67
1:A:475:ILE:HG23	1:A:476:PRO:HD2	1.75	0.67
1:A:305:PHE:CD1	2:A:1240:HOH:O	2.46	0.67
1:A:74:GLN:OE1	1:A:122:SER:HB2	1.95	0.67
1:A:213:ARG:NH2	1:A:236:GLU:OE1	2.25	0.66
1:A:351:GLN:CG	2:A:1279:HOH:O	2.43	0.66
1:A:459:THR:HB	1:A:482:ASN:HD22	1.61	0.65
1:A:167:LYS:HD3	1:A:351:GLN:NE2	2.12	0.65
1:A:268:GLY:HA2	1:A:269:LYS:HB3	1.69	0.65
1:A:334:ARG:NH1	2:A:1009:HOH:O	2.28	0.64
1:A:169:LEU:HD12	1:A:174:GLU:HG2	1.79	0.63
1:A:7:SER:OG	1:A:7:SER:O	2.14	0.63
1:A:149:TRP:HE3	2:A:1108:HOH:O	1.82	0.62
1:A:351:GLN:HG2	2:A:1279:HOH:O	1.99	0.62
1:A:475:ILE:CG2	1:A:476:PRO:HD2	2.29	0.62
1:A:249:ARG:HG2	1:A:305:PHE:CB	2.21	0.61
1:A:395:VAL:HG22	1:A:401:LEU:CD2	2.32	0.60
1:A:284:GLU:H	1:A:287:GLN:NE2	1.99	0.59
1:A:98:LEU:HD23	1:A:106:PHE:HE1	1.68	0.59
1:A:290:LYS:HD2	2:A:1184:HOH:O	2.01	0.59
1:A:267:LYS:O	1:A:269:LYS:CG	2.51	0.58
1:A:144:LYS:HB2	1:A:151:TYR:CE1	2.39	0.58
1:A:180:GLU:HB2	2:A:1278:HOH:O	2.02	0.57
1:A:100:VAL:O	1:A:389:ARG:HG2	2.05	0.57
1:A:267:LYS:O	1:A:269:LYS:CB	2.53	0.56
1:A:351:GLN:CB	2:A:1279:HOH:O	2.31	0.55
1:A:270:ASP:CG	1:A:270:ASP:O	2.45	0.55
1:A:415:ASP:HB3	1:A:445:THR:HG23	1.88	0.55
1:A:98:LEU:HD23	1:A:106:PHE:CE1	2.42	0.54
1:A:6:LYS:HA	1:A:7:SER:C	2.28	0.54
1:A:459:THR:HB	1:A:482:ASN:ND2	2.24	0.52
1:A:467:THR:HG22	2:A:1236:HOH:O	2.10	0.52
1:A:74:GLN:HG2	2:A:1225:HOH:O	2.08	0.52
1:A:79:LEU:HD12	1:A:80:LYS:N	2.25	0.51
1:A:271:GLY:CA	1:A:273:PRO:HD3	2.40	0.51
1:A:461:THR:O	1:A:483:ASP:HA	2.10	0.51
1:A:191:LEU:HB2	2:A:1182:HOH:O	2.12	0.50
1:A:153:VAL:HB	1:A:157:GLU:HB2	1.92	0.49
1:A:74:GLN:CG	2:A:1225:HOH:O	2.61	0.48
1:A:178:TRP:HZ3	1:A:347:PRO:HD3	1.79	0.48
1:A:74:GLN:OE1	1:A:122:SER:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:O	1:A:37:VAL:HG23	2.15	0.47
1:A:81:LEU:HD11	1:A:356:MET:SD	2.55	0.46
1:A:270:ASP:O	1:A:270:ASP:OD2	2.34	0.46
1:A:133:PHE:CD2	2:A:1092:HOH:O	2.64	0.46
1:A:235:MET:HG2	1:A:240:ILE:HB	1.97	0.46
1:A:395:VAL:HG22	1:A:401:LEU:HD21	1.96	0.45
1:A:267:LYS:C	1:A:269:LYS:HB2	2.37	0.45
1:A:482:ASN:OD1	1:A:483:ASP:HB2	2.17	0.45
1:A:25:ASN:ND2	1:A:27:ALA:H	2.15	0.44
1:A:6:LYS:HA	1:A:8:LEU:H	1.81	0.44
1:A:65:THR:HG23	2:A:1111:HOH:O	2.17	0.44
1:A:267:LYS:HG2	1:A:268:GLY:N	2.32	0.44
1:A:271:GLY:HA3	1:A:273:PRO:HD3	1.99	0.43
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.76	0.43
1:A:116:TYR:HA	2:A:1063:HOH:O	2.18	0.43
1:A:170:GLN:HG2	1:A:350:TYR:CZ	2.54	0.42
1:A:251:GLU:HB3	2:A:1306:HOH:O	2.19	0.42
1:A:415:ASP:HB3	1:A:445:THR:HA	2.00	0.42
1:A:343:ASN:O	1:A:346:SER:OG	2.34	0.42
1:A:176:ALA:O	1:A:185:GLU:HG2	2.21	0.41
1:A:404:ASP:OD1	1:A:405:ASP:N	2.53	0.41
1:A:182:PRO:O	1:A:185:GLU:HB2	2.21	0.41
1:A:287:GLN:NE2	2:A:1101:HOH:O	2.51	0.41
1:A:271:GLY:C	1:A:273:PRO:CD	2.82	0.41
1:A:167:LYS:HD3	1:A:351:GLN:HE21	1.85	0.40
1:A:457:VAL:C	1:A:458:LEU:HD12	2.42	0.40
1:A:458:LEU:N	1:A:458:LEU:CD1	2.84	0.40
1:A:453:GLY:H	1:A:456:ASN:ND2	2.19	0.40
1:A:482:ASN:O	1:A:484:THR:HG22	2.20	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	483/505 (96%)	473 (98%)	7 (1%)	3 (1%)	28	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	273	PRO
1	A	189	PRO

### 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	412/432 (95%)	384 (93%)	28 (7%)	18	20

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	6	LYS
1	A	17	LYS
1	A	23	LYS
1	A	49	ASP
1	A	73	LEU
1	A	74	GLN
1	A	79	LEU
1	A	118	ARG
1	A	130	MET
1	A	138	SER
1	A	141	SER
1	A	194	ILE
1	A	251	GLU
1	A	269	LYS
1	A	272	GLN
1	A	281	LEU
1	A	284	GLU

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Mol	Chain	Res	Type
1	A	290	LYS
1	A	301	LYS
1	A	337	LYS
1	A	341	SER
1	A	346	SER
1	A	351	GLN
1	A	403	LEU
1	A	440	GLU
1	A	442	LYS
1	A	484	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	113	GLN
1	A	170	GLN
1	A	219	ASN
1	A	287	GLN
1	A	309	ASN
1	A	322	GLN
1	A	351	GLN
1	A	456	ASN

### 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	485/505 (96%)	-0.04	19 (3%)	40 52	16, 33, 62, 120	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ASP	10.7
1	A	271	GLY	8.9
1	A	269	LYS	6.7
1	A	272	GLN	6.4
1	A	5	MET	5.6
1	A	273	PRO	5.1
1	A	4	ASP	5.0
1	A	342	SER	4.6
1	A	179	ALA	3.8
1	A	343	ASN	3.3
1	A	274	ASP	3.2
1	A	133	PHE	2.9
1	A	344	SER	2.9
1	A	482	ASN	2.4
1	A	168	ILE	2.4
1	A	341	SER	2.3
1	A	405	ASP	2.3
1	A	345	ALA	2.1
1	A	7	SER	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.