



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:21 PM GMT

PDB ID : 3U5T  
Title : The crystal structure of 3-oxoacyl-[acyl-carrier-protein]reductase from *Sinorhizobium meliloti*  
Authors : Zhang, Z.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2011-10-11  
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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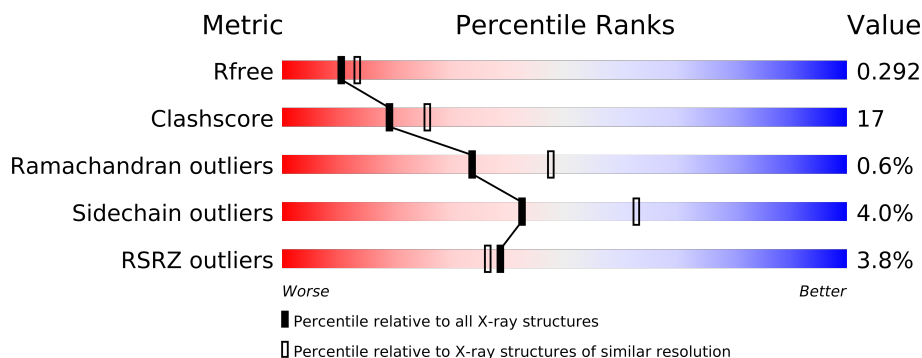
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	267	
1	B	267	
1	C	267	
1	D	267	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6619 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-oxoacyl-[acyl-carrier-protein]reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	Se	0	0	0
			1649	1034	303	309	3			
1	B	233	Total	C	N	O	Se	0	0	0
			1672	1048	306	315	3			
1	C	214	Total	C	N	O	Se	0	0	0
			1534	965	278	288	3			
1	D	228	Total	C	N	O	Se	0	0	0
			1636	1027	300	306	3			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP Q92W70
A	-21	HIS	-	EXPRESSION TAG	UNP Q92W70
A	-20	HIS	-	EXPRESSION TAG	UNP Q92W70
A	-19	HIS	-	EXPRESSION TAG	UNP Q92W70
A	-18	HIS	-	EXPRESSION TAG	UNP Q92W70
A	-17	HIS	-	EXPRESSION TAG	UNP Q92W70
A	-16	HIS	-	EXPRESSION TAG	UNP Q92W70
A	-15	SER	-	EXPRESSION TAG	UNP Q92W70
A	-14	SER	-	EXPRESSION TAG	UNP Q92W70
A	-13	GLY	-	EXPRESSION TAG	UNP Q92W70
A	-12	VAL	-	EXPRESSION TAG	UNP Q92W70
A	-11	ASP	-	EXPRESSION TAG	UNP Q92W70
A	-10	LEU	-	EXPRESSION TAG	UNP Q92W70
A	-9	GLY	-	EXPRESSION TAG	UNP Q92W70
A	-8	THR	-	EXPRESSION TAG	UNP Q92W70
A	-7	GLU	-	EXPRESSION TAG	UNP Q92W70
A	-6	ASN	-	EXPRESSION TAG	UNP Q92W70
A	-5	LEU	-	EXPRESSION TAG	UNP Q92W70
A	-4	TYR	-	EXPRESSION TAG	UNP Q92W70
A	-3	PHE	-	EXPRESSION TAG	UNP Q92W70
A	-2	GLN	-	EXPRESSION TAG	UNP Q92W70

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q92W70
A	0	MSE	-	EXPRESSION TAG	UNP Q92W70
B	-22	MSE	-	EXPRESSION TAG	UNP Q92W70
B	-21	HIS	-	EXPRESSION TAG	UNP Q92W70
B	-20	HIS	-	EXPRESSION TAG	UNP Q92W70
B	-19	HIS	-	EXPRESSION TAG	UNP Q92W70
B	-18	HIS	-	EXPRESSION TAG	UNP Q92W70
B	-17	HIS	-	EXPRESSION TAG	UNP Q92W70
B	-16	HIS	-	EXPRESSION TAG	UNP Q92W70
B	-15	SER	-	EXPRESSION TAG	UNP Q92W70
B	-14	SER	-	EXPRESSION TAG	UNP Q92W70
B	-13	GLY	-	EXPRESSION TAG	UNP Q92W70
B	-12	VAL	-	EXPRESSION TAG	UNP Q92W70
B	-11	ASP	-	EXPRESSION TAG	UNP Q92W70
B	-10	LEU	-	EXPRESSION TAG	UNP Q92W70
B	-9	GLY	-	EXPRESSION TAG	UNP Q92W70
B	-8	THR	-	EXPRESSION TAG	UNP Q92W70
B	-7	GLU	-	EXPRESSION TAG	UNP Q92W70
B	-6	ASN	-	EXPRESSION TAG	UNP Q92W70
B	-5	LEU	-	EXPRESSION TAG	UNP Q92W70
B	-4	TYR	-	EXPRESSION TAG	UNP Q92W70
B	-3	PHE	-	EXPRESSION TAG	UNP Q92W70
B	-2	GLN	-	EXPRESSION TAG	UNP Q92W70
B	-1	SER	-	EXPRESSION TAG	UNP Q92W70
B	0	MSE	-	EXPRESSION TAG	UNP Q92W70
C	-22	MSE	-	EXPRESSION TAG	UNP Q92W70
C	-21	HIS	-	EXPRESSION TAG	UNP Q92W70
C	-20	HIS	-	EXPRESSION TAG	UNP Q92W70
C	-19	HIS	-	EXPRESSION TAG	UNP Q92W70
C	-18	HIS	-	EXPRESSION TAG	UNP Q92W70
C	-17	HIS	-	EXPRESSION TAG	UNP Q92W70
C	-16	HIS	-	EXPRESSION TAG	UNP Q92W70
C	-15	SER	-	EXPRESSION TAG	UNP Q92W70
C	-14	SER	-	EXPRESSION TAG	UNP Q92W70
C	-13	GLY	-	EXPRESSION TAG	UNP Q92W70
C	-12	VAL	-	EXPRESSION TAG	UNP Q92W70
C	-11	ASP	-	EXPRESSION TAG	UNP Q92W70
C	-10	LEU	-	EXPRESSION TAG	UNP Q92W70
C	-9	GLY	-	EXPRESSION TAG	UNP Q92W70
C	-8	THR	-	EXPRESSION TAG	UNP Q92W70
C	-7	GLU	-	EXPRESSION TAG	UNP Q92W70
C	-6	ASN	-	EXPRESSION TAG	UNP Q92W70

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	EXPRESSION TAG	UNP Q92W70
C	-4	TYR	-	EXPRESSION TAG	UNP Q92W70
C	-3	PHE	-	EXPRESSION TAG	UNP Q92W70
C	-2	GLN	-	EXPRESSION TAG	UNP Q92W70
C	-1	SER	-	EXPRESSION TAG	UNP Q92W70
C	0	MSE	-	EXPRESSION TAG	UNP Q92W70
D	-22	MSE	-	EXPRESSION TAG	UNP Q92W70
D	-21	HIS	-	EXPRESSION TAG	UNP Q92W70
D	-20	HIS	-	EXPRESSION TAG	UNP Q92W70
D	-19	HIS	-	EXPRESSION TAG	UNP Q92W70
D	-18	HIS	-	EXPRESSION TAG	UNP Q92W70
D	-17	HIS	-	EXPRESSION TAG	UNP Q92W70
D	-16	HIS	-	EXPRESSION TAG	UNP Q92W70
D	-15	SER	-	EXPRESSION TAG	UNP Q92W70
D	-14	SER	-	EXPRESSION TAG	UNP Q92W70
D	-13	GLY	-	EXPRESSION TAG	UNP Q92W70
D	-12	VAL	-	EXPRESSION TAG	UNP Q92W70
D	-11	ASP	-	EXPRESSION TAG	UNP Q92W70
D	-10	LEU	-	EXPRESSION TAG	UNP Q92W70
D	-9	GLY	-	EXPRESSION TAG	UNP Q92W70
D	-8	THR	-	EXPRESSION TAG	UNP Q92W70
D	-7	GLU	-	EXPRESSION TAG	UNP Q92W70
D	-6	ASN	-	EXPRESSION TAG	UNP Q92W70
D	-5	LEU	-	EXPRESSION TAG	UNP Q92W70
D	-4	TYR	-	EXPRESSION TAG	UNP Q92W70
D	-3	PHE	-	EXPRESSION TAG	UNP Q92W70
D	-2	GLN	-	EXPRESSION TAG	UNP Q92W70
D	-1	SER	-	EXPRESSION TAG	UNP Q92W70
D	0	MSE	-	EXPRESSION TAG	UNP Q92W70

- Molecule 2 is water.

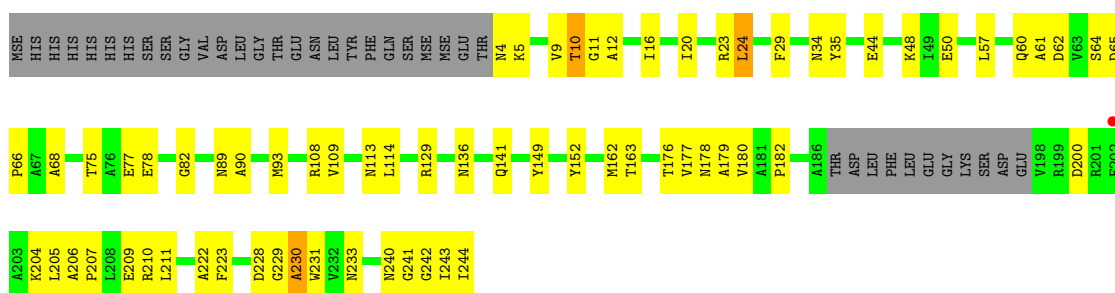
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	47	Total O 47 47	0	0
2	C	11	Total O 11 11	0	0
2	D	37	Total O 37 37	0	0

### 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 errors 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.

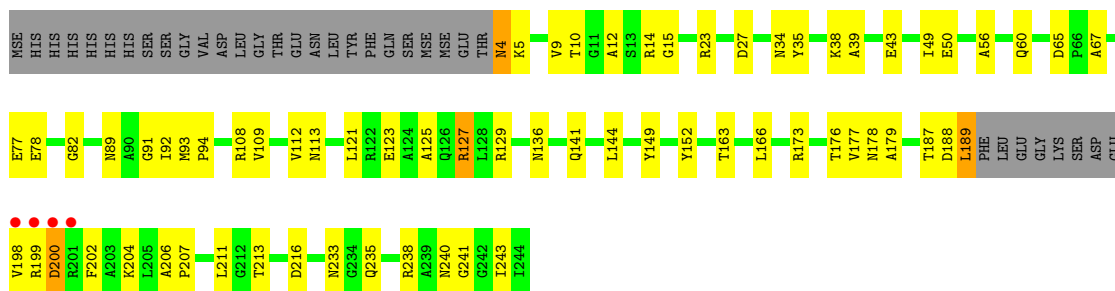
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]reductase

Chain A:



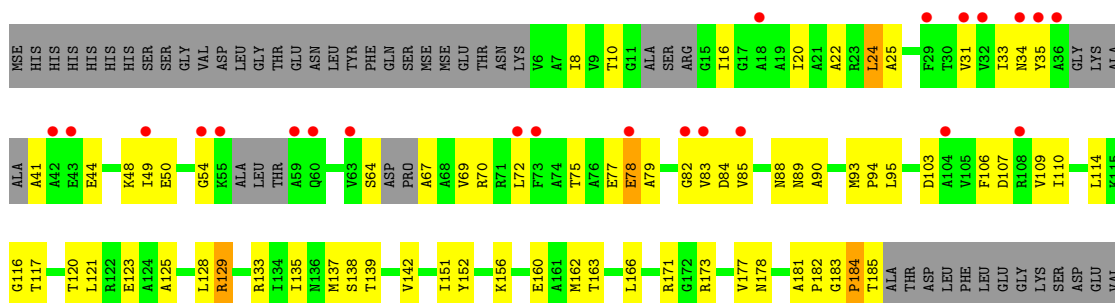
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]reductase

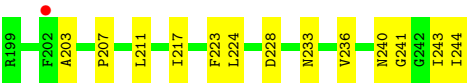
Chain B:



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]reductase

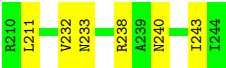
Chain C:





● Molecule 1: 3-oxoacyl-[acyl-carrier-protein]reductase

Chain D: A horizontal bar chart for Chain D showing validation metrics across the full sequence. The bar is primarily green, with a yellow segment in the middle and a grey segment at the end.



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.17Å 95.40Å 112.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.40 48.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.4 (48.22-2.40) 97.4 (48.22-2.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.17 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.244 , 0.285 0.247 , 0.292	Depositor DCC
$R_{free}$ test set	1960 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.4	EDS
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38914 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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	0.44	0/1666	0.57	0/2256
1	B	0.44	0/1689	0.57	0/2288
1	C	0.32	0/1546	0.50	0/2088
1	D	0.37	0/1653	0.53	0/2238
All	All	0.40	0/6554	0.54	0/8870

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1649	0	1692	56	0
1	B	1672	0	1714	58	0
1	C	1534	0	1561	76	0
1	D	1636	0	1681	34	0
2	A	33	0	0	2	0
2	B	47	0	0	4	0
2	C	11	0	0	0	0
2	D	37	0	0	0	0
All	All	6619	0	6648	217	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

The worst 5 of 217 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:VAL:HG12	1:C:123:GLU:HG3	1.51	0.92
1:A:223:PHE:CE1	1:A:228:ASP:O	2.24	0.91
1:A:176:THR:HB	1:A:233:ASN:HB3	1.56	0.88
1:B:93:MSE:HE3	1:B:152:TYR:CE2	2.12	0.85
1:D:178:ASN:OD1	1:D:233:ASN:HA	1.78	0.83

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	226/267 (85%)	215 (95%)	8 (4%)	3 (1%)	18	24
1	B	229/267 (86%)	215 (94%)	13 (6%)	1 (0%)	43	61
1	C	202/267 (76%)	177 (88%)	24 (12%)	1 (0%)	38	53
1	D	224/267 (84%)	211 (94%)	13 (6%)	0	100	100
All	All	881/1068 (82%)	818 (93%)	58 (7%)	5 (1%)	33	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ALA
1	A	78	GLU
1	B	200	ASP
1	A	61	ALA
1	C	184	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	158/186 (85%)	151 (96%)	7 (4%)	39	58
1	B	161/186 (87%)	153 (95%)	8 (5%)	34	51
1	C	147/186 (79%)	140 (95%)	7 (5%)	35	53
1	D	157/186 (84%)	154 (98%)	3 (2%)	69	87
All	All	623/744 (84%)	598 (96%)	25 (4%)	42	63

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	ARG
1	B	204	LYS
1	D	78	GLU
1	B	189	LEU
1	B	211	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	ASN
1	D	34	ASN
1	B	126	GLN
1	B	4	ASN
1	C	89	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

### 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	230/267 (86%)	-0.19	1 (0%) 90 90	30, 42, 59, 99	0
1	B	233/267 (87%)	-0.17	4 (1%) 67 65	24, 42, 56, 65	0
1	C	214/267 (80%)	0.63	24 (11%) 6 5	41, 60, 87, 92	0
1	D	228/267 (85%)	0.05	5 (2%) 59 57	29, 45, 73, 91	0
All	All	905/1068 (84%)	0.07	34 (3%) 38 36	24, 46, 78, 99	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	VAL	4.5
1	C	82	GLY	3.8
1	D	51	ALA	3.6
1	D	200	ASP	3.5
1	B	199	ARG	3.5

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.