



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:48 am GMT

PDB ID : 2EC5
Title : Crystal structures reveal a thiol-protease like catalytic triad in the C-terminal region of Pasteurella multocida toxin
Authors : Kitadokoro, K.; Horiguchi, Y.; Kamitani, S.
Deposited on : 2007-02-09
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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.

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

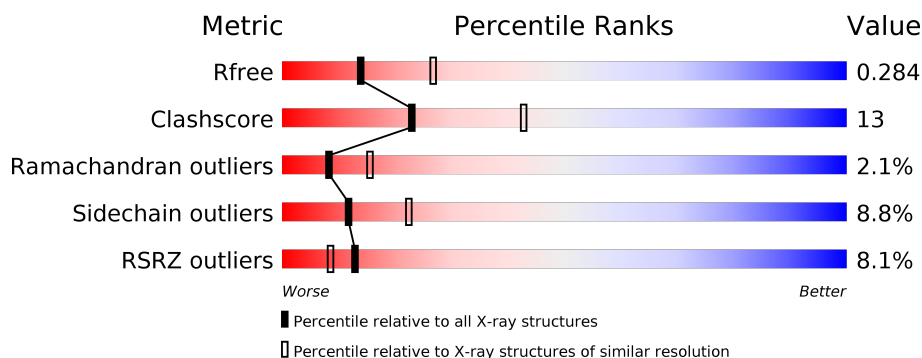
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 ≥ 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	746	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	B	746	<div> <div>8%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11528 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 Dermonecrotic toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5643	3603	939	1075	26			
1	B	711	Total	C	N	O	S	0	0	0
			5643	3603	939	1075	26			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	MET	-	CLONING ARTIFACT	UNP P17452
A	541	GLY	-	CLONING ARTIFACT	UNP P17452
A	542	HIS	-	EXPRESSION TAG	UNP P17452
A	543	HIS	-	EXPRESSION TAG	UNP P17452
A	544	HIS	-	EXPRESSION TAG	UNP P17452
A	545	HIS	-	EXPRESSION TAG	UNP P17452
A	546	HIS	-	EXPRESSION TAG	UNP P17452
A	547	HIS	-	EXPRESSION TAG	UNP P17452
A	548	ASP	-	CLONING ARTIFACT	UNP P17452
A	549	TYR	-	CLONING ARTIFACT	UNP P17452
A	550	ASP	-	CLONING ARTIFACT	UNP P17452
A	551	ILE	-	CLONING ARTIFACT	UNP P17452
A	552	PRO	-	CLONING ARTIFACT	UNP P17452
A	553	THR	-	CLONING ARTIFACT	UNP P17452
A	554	THR	-	CLONING ARTIFACT	UNP P17452
A	555	GLU	-	CLONING ARTIFACT	UNP P17452
A	556	ASN	-	CLONING ARTIFACT	UNP P17452
A	557	LEU	-	CLONING ARTIFACT	UNP P17452
A	558	TYR	-	CLONING ARTIFACT	UNP P17452
A	559	PHE	-	CLONING ARTIFACT	UNP P17452
A	560	GLN	-	CLONING ARTIFACT	UNP P17452
A	561	GLY	-	CLONING ARTIFACT	UNP P17452
A	562	ALA	-	CLONING ARTIFACT	UNP P17452
A	563	HIS	-	CLONING ARTIFACT	UNP P17452
A	564	MET	-	CLONING ARTIFACT	UNP P17452

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Chain	Residue	Modelled	Actual	Comment	Reference
A	565	GLY	-	CLONING ARTIFACT	UNP P17452
A	566	ILE	-	CLONING ARTIFACT	UNP P17452
A	567	GLN	-	CLONING ARTIFACT	UNP P17452
A	568	ARG	-	CLONING ARTIFACT	UNP P17452
A	1159	SER	CYS	ENGINEERED	UNP P17452
B	540	MET	-	CLONING ARTIFACT	UNP P17452
B	541	GLY	-	CLONING ARTIFACT	UNP P17452
B	542	HIS	-	EXPRESSION TAG	UNP P17452
B	543	HIS	-	EXPRESSION TAG	UNP P17452
B	544	HIS	-	EXPRESSION TAG	UNP P17452
B	545	HIS	-	EXPRESSION TAG	UNP P17452
B	546	HIS	-	EXPRESSION TAG	UNP P17452
B	547	HIS	-	EXPRESSION TAG	UNP P17452
B	548	ASP	-	CLONING ARTIFACT	UNP P17452
B	549	TYR	-	CLONING ARTIFACT	UNP P17452
B	550	ASP	-	CLONING ARTIFACT	UNP P17452
B	551	ILE	-	CLONING ARTIFACT	UNP P17452
B	552	PRO	-	CLONING ARTIFACT	UNP P17452
B	553	THR	-	CLONING ARTIFACT	UNP P17452
B	554	THR	-	CLONING ARTIFACT	UNP P17452
B	555	GLU	-	CLONING ARTIFACT	UNP P17452
B	556	ASN	-	CLONING ARTIFACT	UNP P17452
B	557	LEU	-	CLONING ARTIFACT	UNP P17452
B	558	TYR	-	CLONING ARTIFACT	UNP P17452
B	559	PHE	-	CLONING ARTIFACT	UNP P17452
B	560	GLN	-	CLONING ARTIFACT	UNP P17452
B	561	GLY	-	CLONING ARTIFACT	UNP P17452
B	562	ALA	-	CLONING ARTIFACT	UNP P17452
B	563	HIS	-	CLONING ARTIFACT	UNP P17452
B	564	MET	-	CLONING ARTIFACT	UNP P17452
B	565	GLY	-	CLONING ARTIFACT	UNP P17452
B	566	ILE	-	CLONING ARTIFACT	UNP P17452
B	567	GLN	-	CLONING ARTIFACT	UNP P17452
B	568	ARG	-	CLONING ARTIFACT	UNP P17452
B	1159	SER	CYS	ENGINEERED	UNP P17452

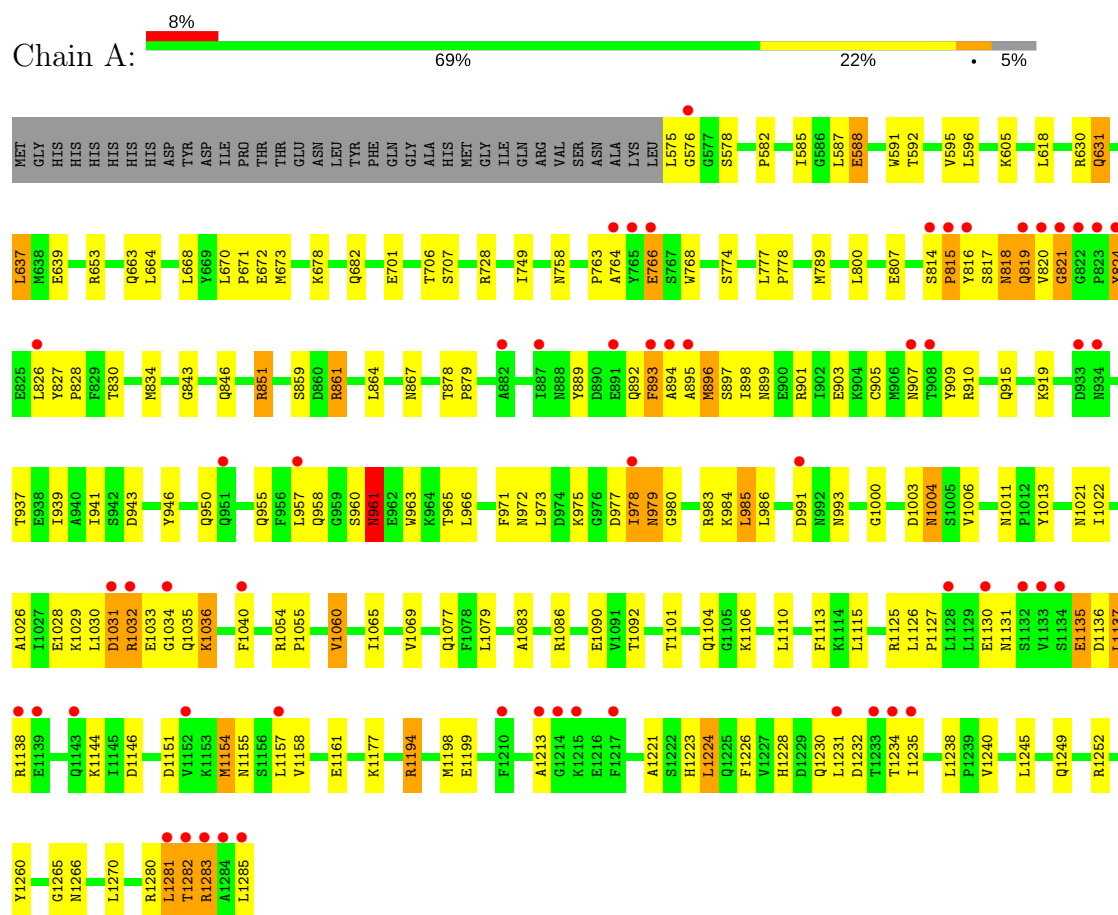
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	119	Total O 119 119	0	0
2	B	123	Total O 123 123	0	0

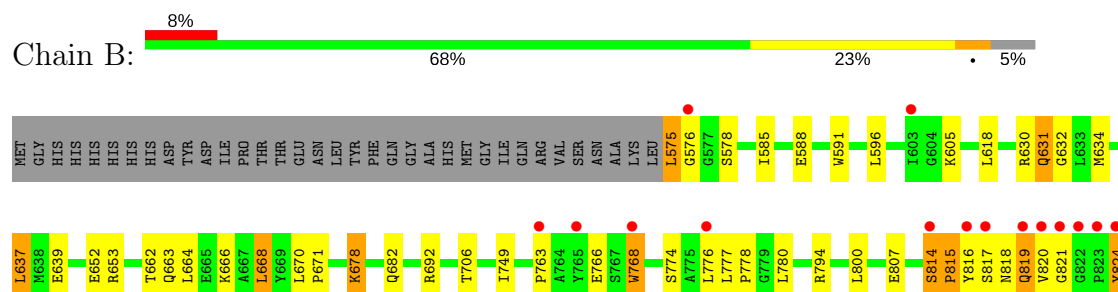
3 Residue-property plots

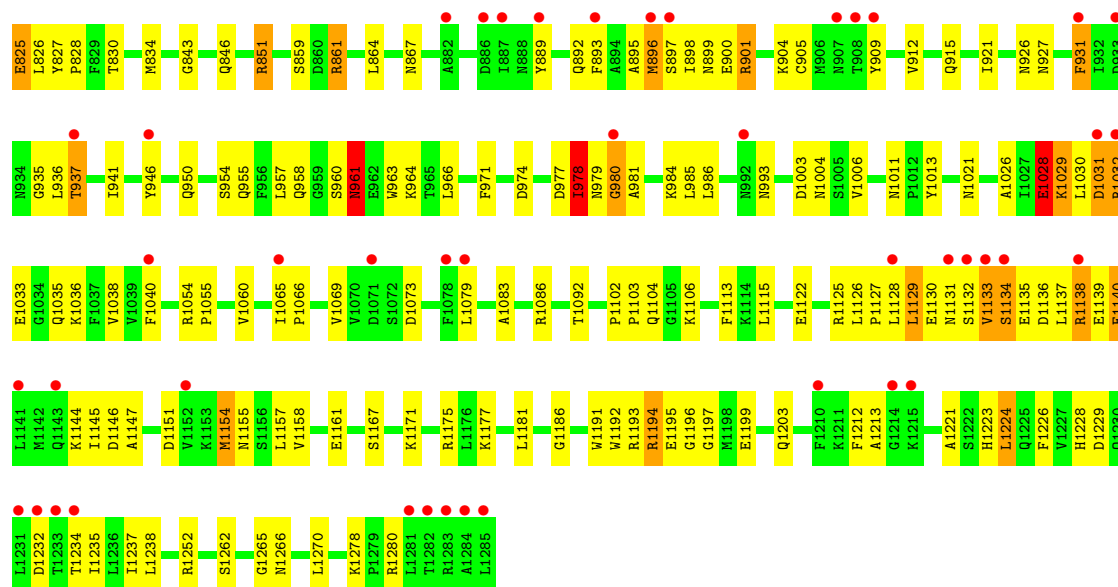
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Dermonecrotic toxin



• Molecule 1: Dermonecrotic toxin





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.36Å 132.82Å 82.55Å 90.00° 114.74° 90.00°	Depositor
Resolution (Å)	44.81 – 2.60 44.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.81-2.60) 97.0 (44.81-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.286 0.230 , 0.284	Depositor DCC
R_{free} test set	2921 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.478 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11528	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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

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	0.41	0/5769	0.59	0/7811
1	B	0.46	2/5769 (0.0%)	0.60	2/7811 (0.0%)
All	All	0.44	2/11538 (0.0%)	0.60	2/15622 (0.0%)

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	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	926	ASN	CG-ND2	7.94	1.52	1.32
1	B	926	ASN	CG-OD1	6.53	1.38	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1073	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	B	1073	ASP	CB-CG-OD1	8.22	125.69	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	824	TYR	Peptide
1	B	824	TYR	Peptide

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	5643	0	5575	137	0
1	B	5643	0	5575	153	0
2	A	119	0	0	6	0
2	B	123	0	0	4	0
All	All	11528	0	11150	289	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 13.

The worst 5 of 289 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:B:1129:LEU:CB	1:B:1130:GLU:HA	1.66	1.22
1:B:1129:LEU:HB3	1:B:1130:GLU:CA	1.69	1.21
1:B:817:SER:CB	1:B:818:ASN:HA	1.72	1.18
1:B:817:SER:HB3	1:B:818:ASN:HA	1.27	1.15
1:A:893:PHE:HA	1:A:894:ALA:HB2	1.30	1.10

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	709/746 (95%)	647 (91%)	49 (7%)	13 (2%)	10 19
1	B	709/746 (95%)	629 (89%)	63 (9%)	17 (2%)	7 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1418/1492 (95%)	1276 (90%)	112 (8%)	30 (2%)	8	15

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	961	ASN
1	A	978	ILE
1	B	814	SER
1	B	815	PRO
1	B	1133	VAL

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	616/646 (95%)	560 (91%)	56 (9%)	11	21
1	B	616/646 (95%)	563 (91%)	53 (9%)	12	23
All	All	1232/1292 (95%)	1123 (91%)	109 (9%)	12	22

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1224	LEU
1	B	631	GLN
1	B	1154	MET
1	A	1230	GLN
1	A	1285	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1228	HIS
1	B	785	GLN
1	B	1131	ASN

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Mol	Chain	Res	Type
1	B	631	GLN
1	B	818	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 carbohydrates 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	711/746 (95%)	0.61	56 (7%) 13 9	45, 61, 77, 99	0
1	B	711/746 (95%)	0.58	59 (8%) 12 8	38, 52, 69, 95	0
All	All	1422/1492 (95%)	0.60	115 (8%) 13 8	38, 57, 75, 99	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	908	THR	8.2
1	B	576	GLY	7.1
1	B	1133	VAL	6.9
1	A	1284	ALA	6.8
1	A	907	ASN	6.6

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.