wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 11:20 PM EDT

PDB ID	:	5Z00
Title	:	AtVAL1 B3 domain in complex with 15bp-DNA
Authors	:	Wu, B.X.; Zhang, M.M.
Deposited on	:	2017-12-17
Resolution	:	2.59 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
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:

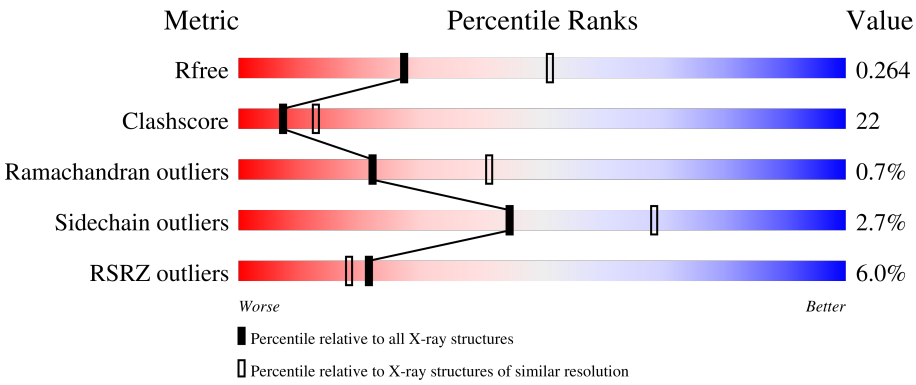
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.59 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	15	33% 53% 13%
1	E	15	13% 20% 53% 27%
1	I	15	7% 27% 73%
2	B	15	20% 47% 33%
2	J	15	13% 87%

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Mol	Chain	Length	Quality of chain
3	C	128	3% 60% 27% 13%
3	G	128	2% 60% 25% • 13%
3	K	128	12% 42% 41% • 13%
3	M	128	3% 54% 31% • 13%
4	F	16	12% 38% 44% 12% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5294 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 DNA chain called DNA (5'-D(*AP*AP*TP*TP*CP*TP*GP*CP*AP*TP*GP*GP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	15	305	148	53	90	14	0	0	0
1	E	15	308	148	53	92	15	0	0	0
1	I	15	305	148	53	90	14	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*AP*TP*CP*CP*AP*TP*GP*CP*AP*GP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	15	304	147	57	86	14	0	0	0
2	J	15	304	147	57	86	14	0	0	0

- Molecule 3 is a protein called B3 domain-containing transcription repressor VAL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	111	866	551	153	156	6	0	0	0
3	G	111	866	551	153	156	6	0	0	0
3	K	111	866	551	153	156	6	0	0	0
3	M	111	866	551	153	156	6	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*AP*AP*TP*CP*CP*AP*TP*GP*CP*AP*GP*AP*AP*TP*T)-3').

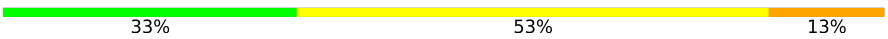
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	F	15	304	147	57	86	14	0	0	0

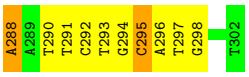
3 Residue-property plots (i)

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: DNA (5'-D(*AP*AP*TP*TP*CP*TP*GP*CP*AP*TP*GP*GP*AP*TP*T)-3')

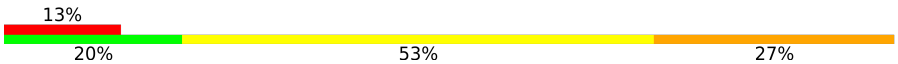
Chain A:





• Molecule 1: DNA (5'-D(*AP*AP*TP*TP*CP*TP*GP*CP*AP*TP*GP*GP*AP*TP*T)-3')

Chain E:

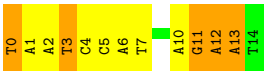


• Molecule 1: DNA (5'-D(*AP*AP*TP*TP*CP*TP*GP*CP*AP*TP*GP*GP*AP*TP*T)-3')

Chain I:

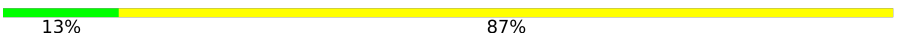
• Molecule 2: DNA (5'-D(*TP*AP*AP*TP*CP*CP*AP*TP*GP*CP*AP*GP*AP*AP*T)-3')

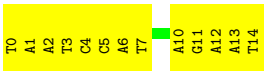
Chain B:



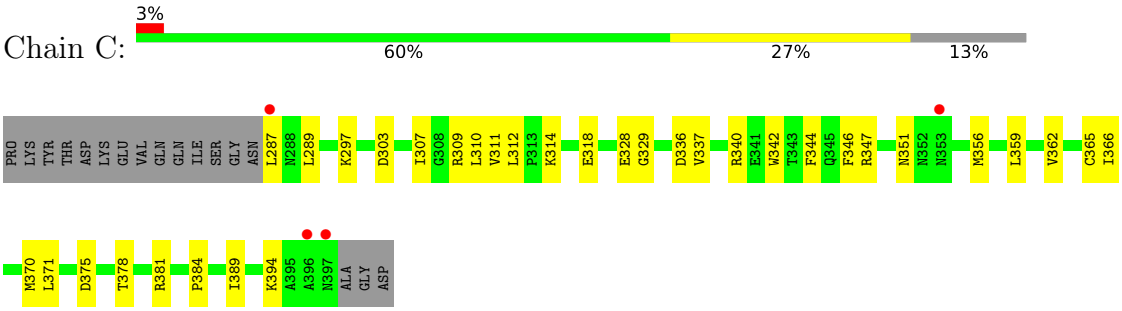
• Molecule 2: DNA (5'-D(*TP*AP*AP*TP*CP*CP*AP*TP*GP*CP*AP*GP*AP*AP*T)-3')

Chain J:

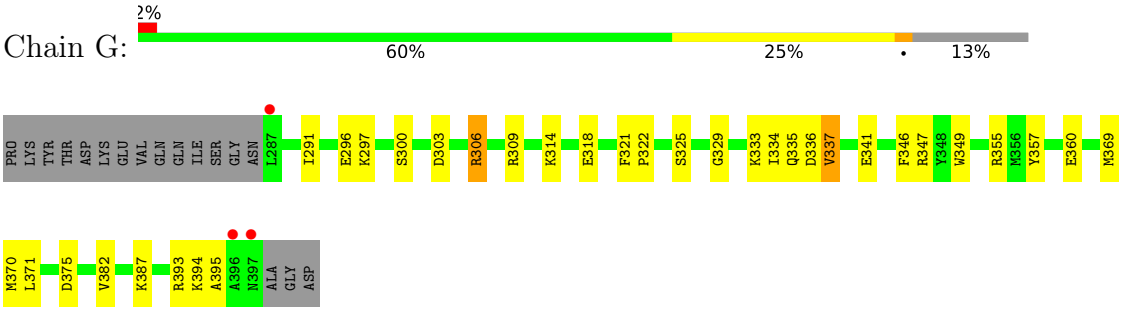




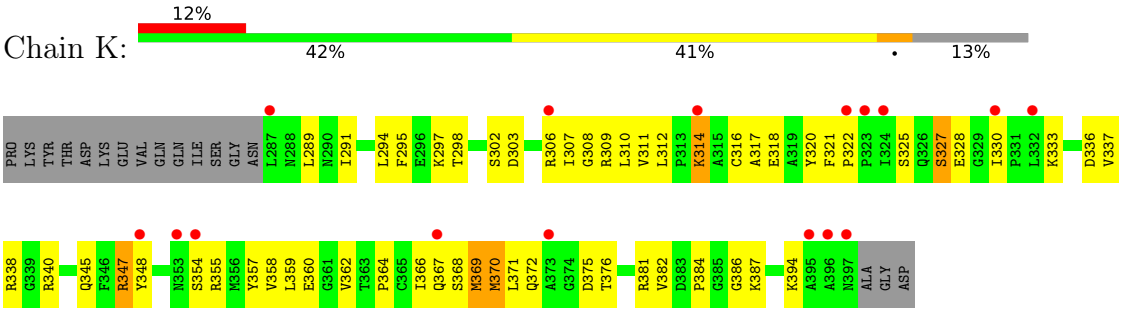
• Molecule 3: B3 domain-containing transcription repressor VAL1



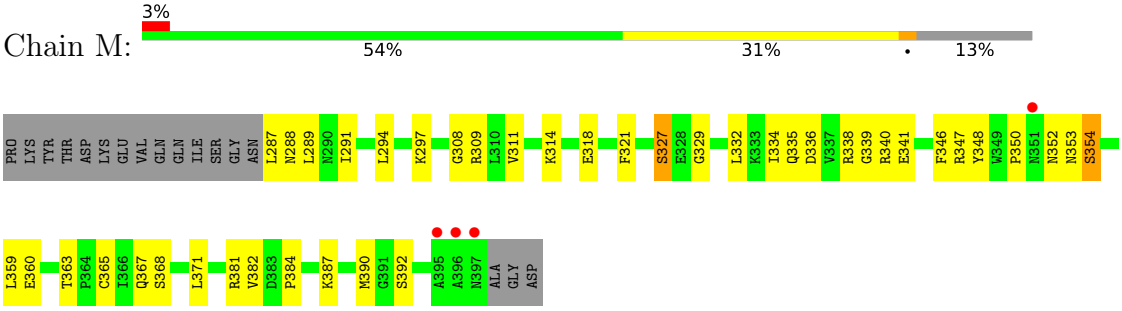
• Molecule 3: B3 domain-containing transcription repressor VAL1



• Molecule 3: B3 domain-containing transcription repressor VAL1

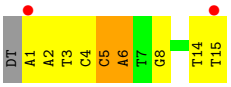


• Molecule 3: B3 domain-containing transcription repressor VAL1



• Molecule 4: DNA (5'-D(*TP*AP*AP*TP*CP*CP*AP*TP*GP*CP*AP*GP*AP*AP*TP*T)-3')

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.22Å 97.42Å 71.15Å 90.00° 110.19° 90.00°	Depositor
Resolution (Å)	29.20 – 2.59 29.20 – 2.59	Depositor EDS
% Data completeness (in resolution range)	77.1 (29.20-2.59) 75.7 (29.20-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.216 , 0.268 0.219 , 0.264	Depositor DCC
R_{free} test set	1013 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5294	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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	1.47	7/341 (2.1%)	0.89	1/525 (0.2%)
1	E	1.07	4/344 (1.2%)	0.88	1/529 (0.2%)
1	I	0.78	0/341	0.95	0/525
2	B	1.49	8/341 (2.3%)	0.92	0/524
2	J	0.93	1/341 (0.3%)	0.92	0/524
3	C	0.63	0/885	0.83	1/1198 (0.1%)
3	G	0.60	0/885	0.82	0/1198
3	K	0.69	0/885	1.06	7/1198 (0.6%)
3	M	0.62	1/885 (0.1%)	0.86	0/1198
4	F	1.36	2/341 (0.6%)	1.08	0/524
All	All	0.89	23/5589 (0.4%)	0.91	10/7943 (0.1%)

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
3	K	0	1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	DT	O3'-P	-9.57	1.49	1.61
2	B	5	DC	O3'-P	-9.17	1.50	1.61
4	F	5	DC	O3'-P	-9.04	1.50	1.61
1	A	292	DC	O3'-P	-7.14	1.52	1.61
4	F	6	DA	O3'-P	-6.68	1.53	1.61

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	347	ARG	NE-CZ-NH1	11.09	125.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	333	LYS	CD-CE-NZ	6.36	126.32	111.70
3	K	347	ARG	NE-CZ-NH2	-6.33	117.14	120.30
3	K	333	LYS	CG-CD-CE	-6.19	93.34	111.90
3	C	347	ARG	NE-CZ-NH1	5.76	123.18	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	367	GLN	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	305	0	173	12	0
1	E	308	0	172	23	0
1	I	305	0	173	21	1
2	B	304	0	171	10	0
2	J	304	0	171	19	1
3	C	866	0	876	26	0
3	G	866	0	876	28	0
3	K	866	0	876	66	0
3	M	866	0	876	31	0
4	F	304	0	171	19	0
All	All	5294	0	4535	217	1

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 22.

The worst 5 of 217 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:E:301:DT:O4	4:F:2:DA:N6	1.65	1.27
1:I:300:DA:N1	2:J:3:DT:O4	1.95	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:DA:N1	4:F:15:DT:N3	2.10	0.99
1:E:289:DA:H61	4:F:14:DT:H3	1.00	0.98
1:E:301:DT:N3	4:F:2:DA:N1	2.12	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:288:DA:N1	2:J:0:DT:O4[2_458]	2.13	0.07

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	
3	C	109/128 (85%)	102 (94%)	7 (6%)	0	100	100
3	G	109/128 (85%)	104 (95%)	5 (5%)	0	100	100
3	K	109/128 (85%)	102 (94%)	5 (5%)	2 (2%)	8	16
3	M	109/128 (85%)	103 (94%)	5 (5%)	1 (1%)	17	34
All	All	436/512 (85%)	411 (94%)	22 (5%)	3 (1%)	22	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	306	ARG
3	K	327	SER
3	M	352	ASN

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	
3	C	94/108 (87%)	92 (98%)	2 (2%)	53	75
3	G	94/108 (87%)	91 (97%)	3 (3%)	39	63
3	K	94/108 (87%)	92 (98%)	2 (2%)	53	75
3	M	94/108 (87%)	91 (97%)	3 (3%)	39	63
All	All	376/432 (87%)	366 (97%)	10 (3%)	44	68

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	327	SER
3	M	353	ASN
3	M	354	SER
3	G	334	ILE
3	G	337	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	290	ASN
3	M	335	GLN

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	15/15 (100%)	-0.51	0 100 100	45, 49, 56, 56	0
1	E	15/15 (100%)	0.66	2 (13%) 3 2	54, 62, 109, 114	0
1	I	15/15 (100%)	0.92	1 (6%) 17 14	84, 94, 107, 112	0
2	B	15/15 (100%)	-0.27	0 100 100	35, 52, 61, 64	0
2	J	15/15 (100%)	0.49	0 100 100	65, 91, 101, 102	0
3	C	111/128 (86%)	0.02	4 (3%) 42 38	20, 33, 53, 92	0
3	G	111/128 (86%)	0.09	3 (2%) 54 51	24, 38, 66, 80	0
3	K	111/128 (86%)	0.81	16 (14%) 2 1	32, 63, 90, 115	0
3	M	111/128 (86%)	0.01	4 (3%) 42 38	19, 34, 66, 111	0
4	F	15/16 (93%)	0.35	2 (13%) 3 2	40, 49, 96, 104	0
All	All	534/603 (88%)	0.24	32 (5%) 21 18	19, 43, 92, 115	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	397	ASN	9.6
3	M	396	ALA	8.6
3	K	396	ALA	8.3
3	K	397	ASN	7.0
3	G	287	LEU	6.2

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.