W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 10:16 pm BST

PDB ID	:	3KYH
Title	:	Saccharomyces cerevisiae Cet1-Ceg1 capping apparatus
Authors	:	Lima, C.D.
Deposited on	:	2009-12-06
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

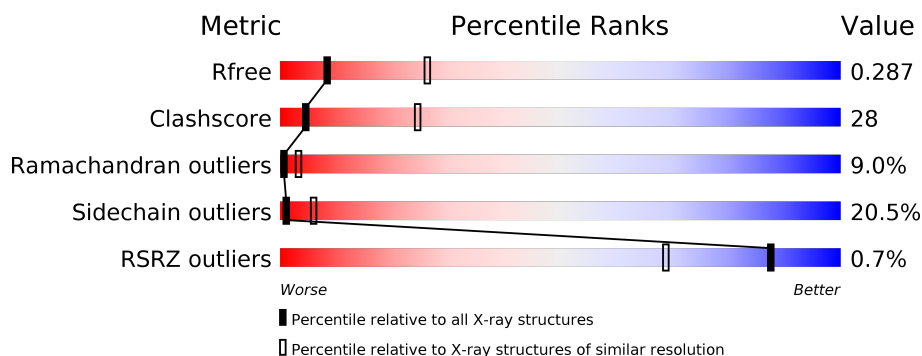|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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	Percentile Ranks	Value
Rfree		0.287
Clashscore		28
Ramachandran outliers		9.0%
Sidechain outliers		20.5%
RSRZ outliers		0.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	310	34% 40% 13% • 11%
1	B	310	37% 40% 10% • 11%
2	C	461	38% 33% 11% • 16%
2	D	461	33% 37% 12% • 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10696 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 mRNA-capping enzyme subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total 2212	C 1407	N 375	O 426	S 4	0	0	0
1	B	276	Total 2212	C 1407	N 375	O 426	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	INITIATING METHIONINE	UNP O13297
B	240	MET	-	INITIATING METHIONINE	UNP O13297

- Molecule 2 is a protein called mRNA-capping enzyme subunit alpha.

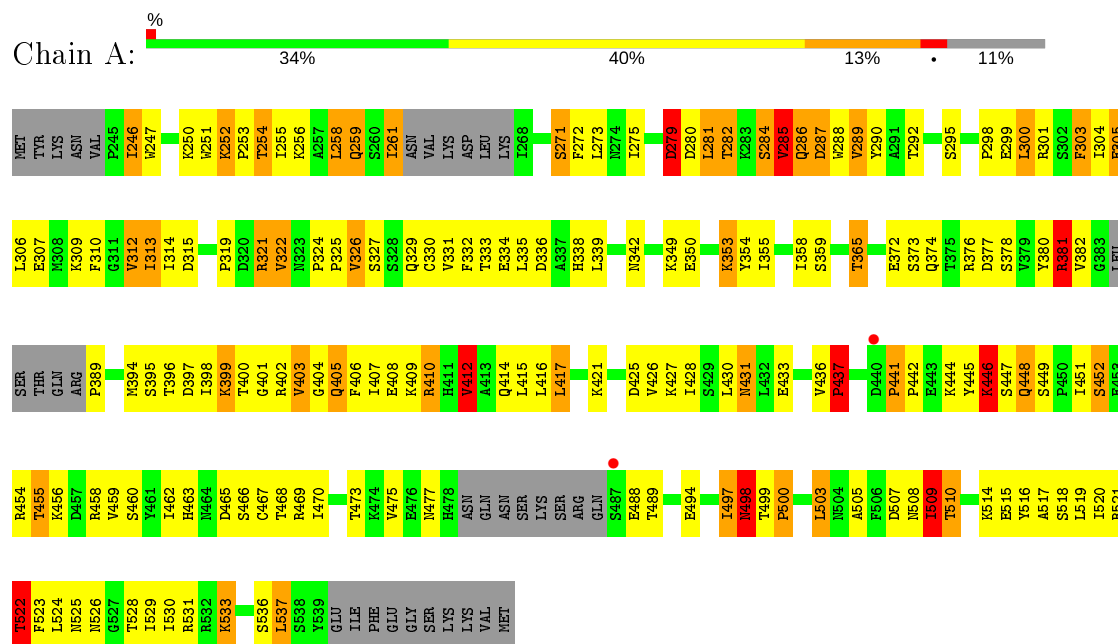| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	387	Total 3136	C 2007	N 528	O 583	S 18	0	0	0
2	D	387	Total 3136	C 2007	N 528	O 583	S 18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

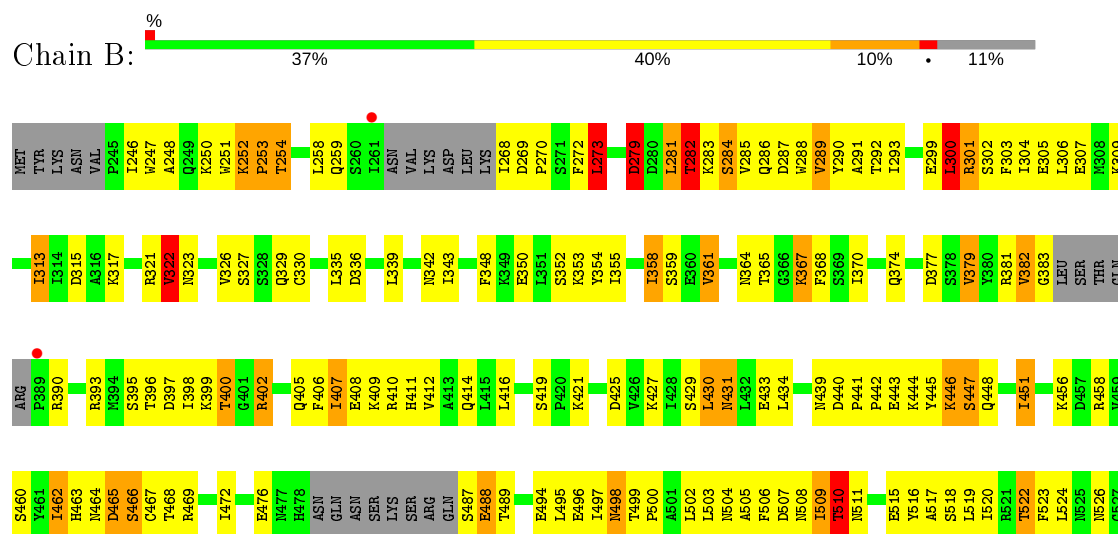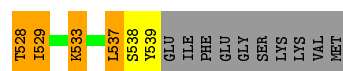| Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP Q01159
C	0	LEU	-	EXPRESSION TAG	UNP Q01159
D	-1	SER	-	EXPRESSION TAG	UNP Q01159
D	0	LEU	-	EXPRESSION TAG	UNP Q01159

3 Residue-property plots (i)

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: mRNA-capping enzyme subunit beta
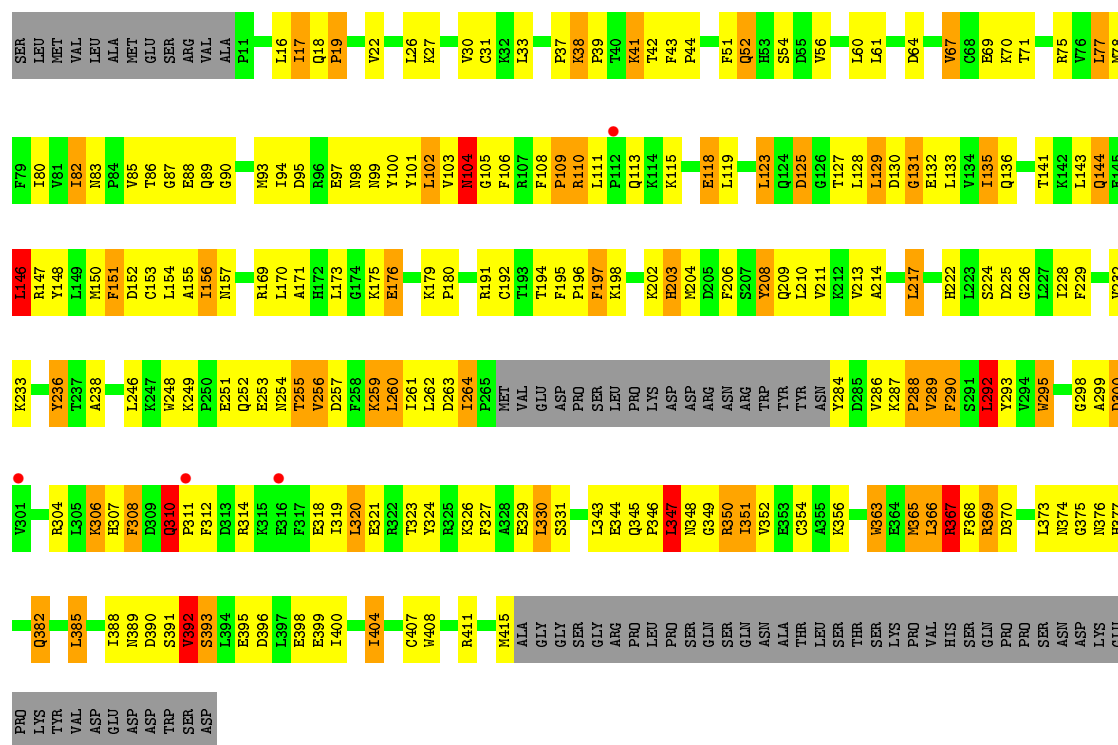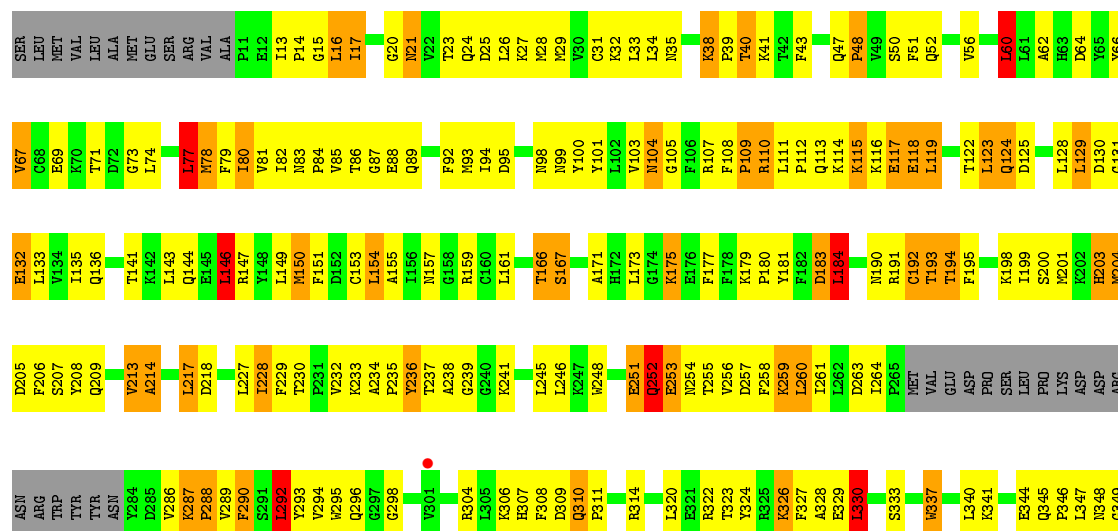

- Molecule 1: mRNA-capping enzyme subunit beta

T528 I529 K533 L537 S538 Y539 GLU ILE PHE GLU GLY SER LYS LYS VAL MET

● Molecule 2: mRNA-capping enzyme subunit alpha

Chain C:

● Molecule 2: mRNA-capping enzyme subunit alpha

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	165.99Å 165.99Å 172.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.98-3.00) 95.3 (19.98-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.249 , 0.298 0.249 , 0.287	Depositor DCC
R_{free} test set	2580 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 22.4	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.458 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.514 for H, K, L 0.486 for h+k,-k,-l	Depositor
Outliers	0 of 50992 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10696	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.92	1/2256 (0.0%)	1.24	10/3058 (0.3%)
1	B	0.99	1/2256 (0.0%)	1.29	14/3058 (0.5%)
2	C	0.67	0/3207	1.04	11/4334 (0.3%)
2	D	0.67	0/3207	1.05	7/4334 (0.2%)
All	All	0.80	2/10926 (0.0%)	1.14	42/14784 (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	1
1	B	0	1
2	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	VAL	CB-CG1	6.55	1.66	1.52
1	B	288	TRP	CE2-CZ2	-5.30	1.30	1.39

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	217	LEU	CA-CB-CG	9.07	136.16	115.30
1	A	458	ARG	NE-CZ-NH1	8.68	124.64	120.30
2	D	385	LEU	CA-CB-CG	7.84	133.32	115.30
2	C	170	LEU	CA-CB-CG	7.33	132.15	115.30
2	D	292	LEU	CA-CB-CG	6.88	131.12	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	ASP	Peptide
1	B	465	ASP	Peptide
2	C	310	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	2212	0	2218	152	0
1	B	2212	0	2218	138	0
2	C	3136	0	3126	156	0
2	D	3136	0	3126	188	0
All	All	10696	0	10688	607	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 28.

The worst 5 of 607 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:446:LYS:NZ	1:B:446:LYS:HA	1.64	1.13
2:D:109:PRO:HD2	2:D:180:PRO:HB2	1.24	1.13
1:B:497:ILE:HD11	1:B:519:LEU:HD11	1.32	1.12
2:C:390:ASP:O	2:C:392:VAL:HG23	1.55	1.07
1:A:499:THR:HG22	1:A:503:LEU:HD12	1.37	1.07

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	268/310 (86%)	195 (73%)	46 (17%)	27 (10%)	0	2
1	B	268/310 (86%)	192 (72%)	48 (18%)	28 (10%)	0	2
2	C	383/461 (83%)	287 (75%)	68 (18%)	28 (7%)	1	5
2	D	383/461 (83%)	280 (73%)	69 (18%)	34 (9%)	1	3
All	All	1302/1542 (84%)	954 (73%)	231 (18%)	117 (9%)	1	3

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASP
1	A	286	GLN
1	A	336	ASP
1	A	342	ASN
1	B	279	ASP

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	254/290 (88%)	203 (80%)	51 (20%)	1	6
1	B	254/290 (88%)	211 (83%)	43 (17%)	2	11
2	C	352/421 (84%)	279 (79%)	73 (21%)	1	6
2	D	352/421 (84%)	270 (77%)	82 (23%)	1	4
All	All	1212/1422 (85%)	963 (80%)	249 (20%)	1	6

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	129	LEU
2	C	290	PHE
2	D	333	SER

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Mol	Chain	Res	Type
2	C	144	GLN
2	C	211	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	83	ASN
2	C	144	GLN
2	D	252	GLN
2	C	89	GLN
2	C	98	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(Å²)	Q<0.9
1	A	276/310 (89%)	-0.25	2 (0%)	87	69	24, 55, 112, 145	0
1	B	276/310 (89%)	-0.26	2 (0%)	87	69	19, 53, 100, 156	0
2	C	387/461 (83%)	-0.11	4 (1%)	82	59	46, 92, 123, 154	0
2	D	387/461 (83%)	-0.17	1 (0%)	94	84	50, 91, 124, 155	0
All	All	1326/1542 (85%)	-0.19	9 (0%)	87	69	19, 80, 121, 156	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	ILE	8.4
1	A	487	SER	6.0
1	A	440	ASP	4.3
2	C	311	PRO	2.6
2	D	301	VAL	2.3

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.