wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	4DJI
Title	:	Structure of glutamate-GABA antiporter GadC
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Deposited on	:	2012-02-02
Resolution	:	3.19 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 following versions of software and data (see references (1)) were used in the production of this report:

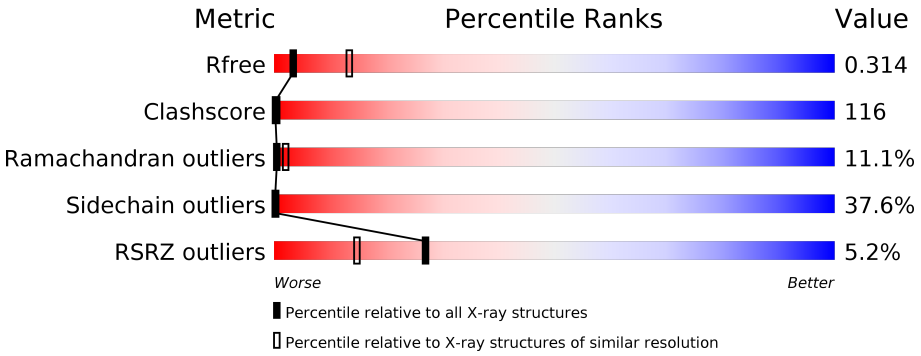
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.19 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	511	4% 14% 49% 29%
1	B	511	6% 13% 50% 28% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7342 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 Probable glutamate/gamma-aminobutyrate antiporter.

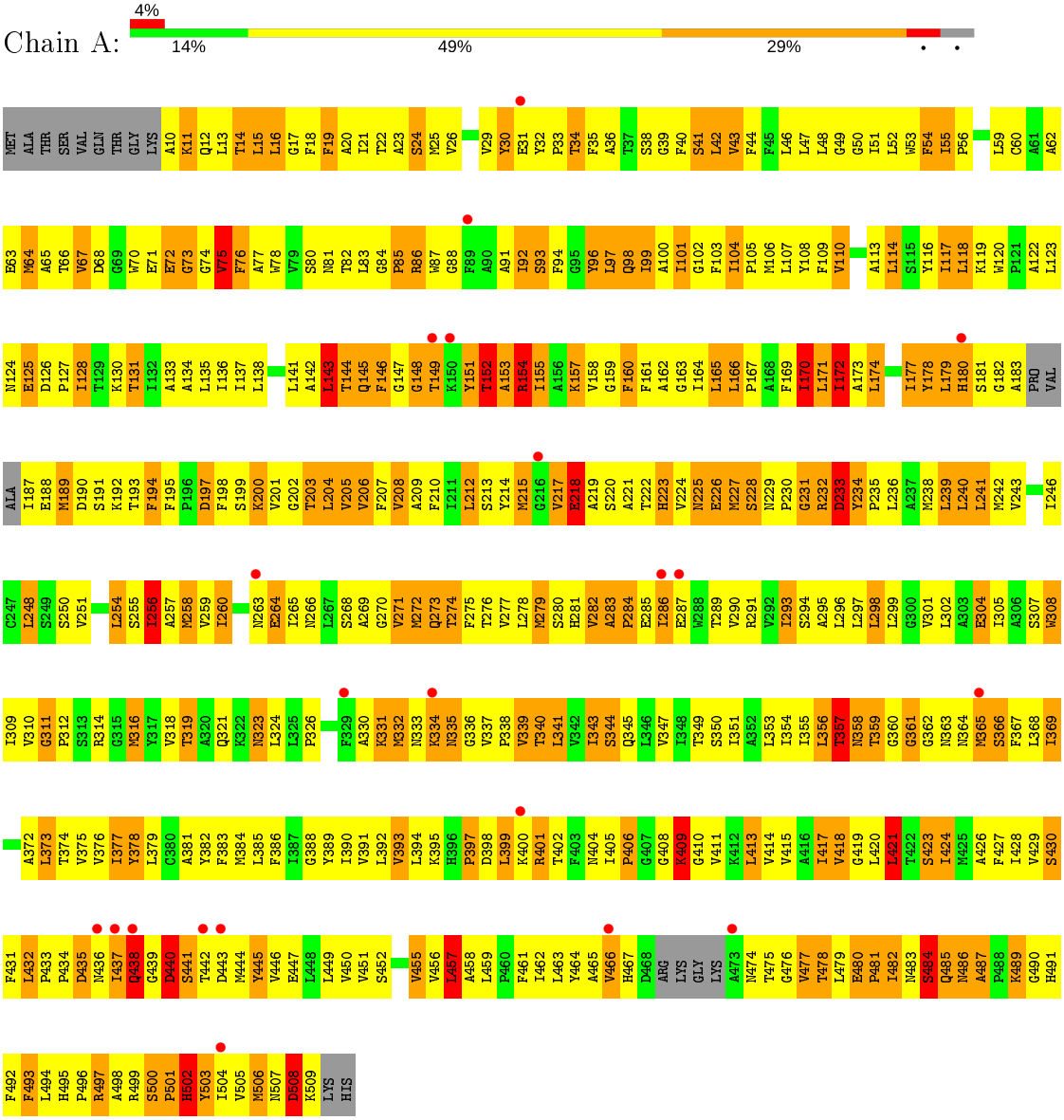
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3732	2493	581	636	22			
1	B	480	Total	C	N	O	S	0	0	0
			3610	2417	556	616	21			

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.

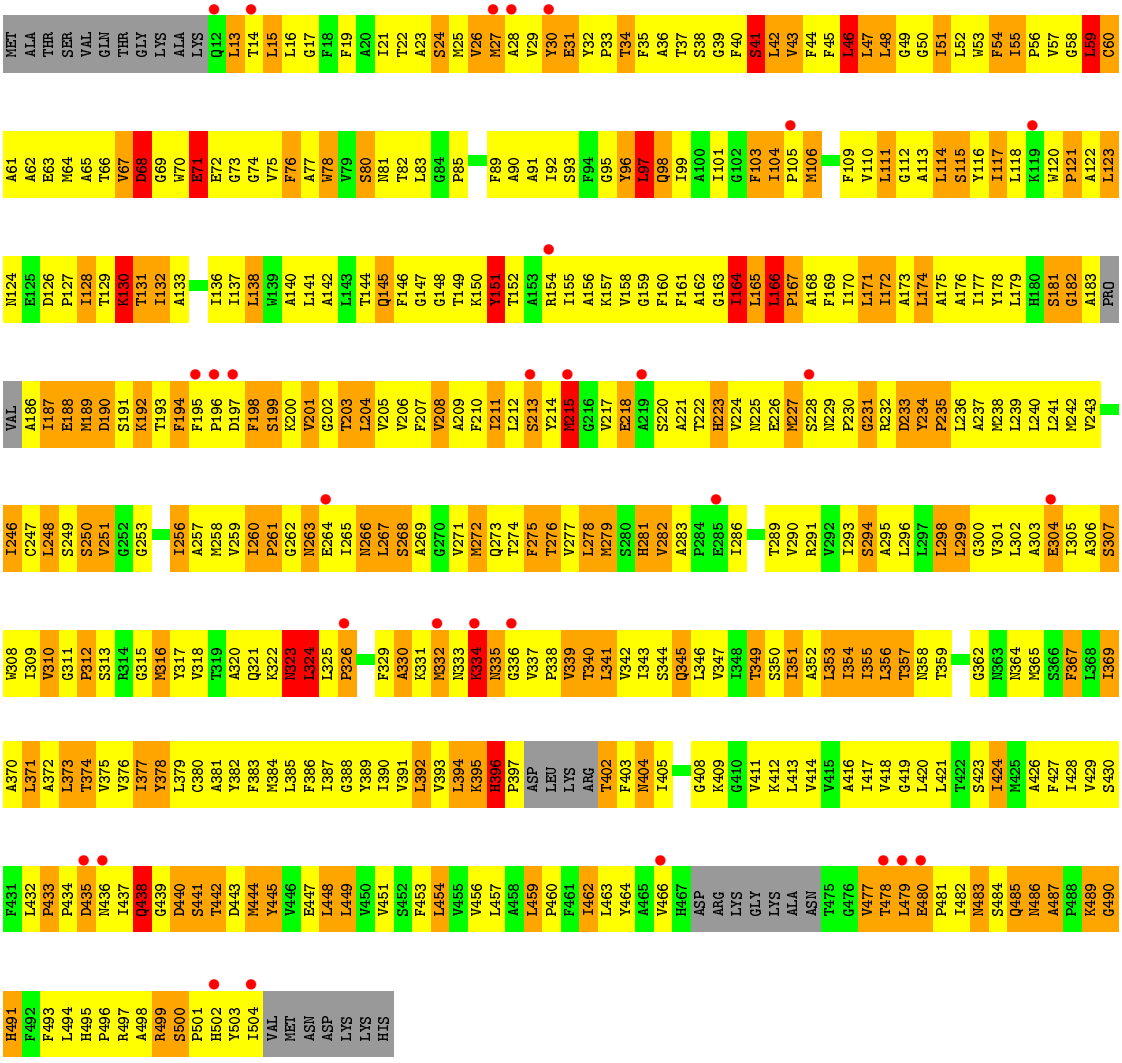
- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter

Chain A:



- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter

Chain B:


MET ALA THR SER VAL GLN THR GLY LYS ALA LYS Q12 L13 T14 L15 L16 G17 F18 F19 A20 I21 T22 A23 S24 M25 V26 M27 A28 V29 Y30 E31 Y32 P33 T34 F35 A36 T37 S38 G39 F40 S41 L42 V43 F44 F45 L46 L47 L48 G49 G50 I51 L52 W53 F54 I55 P56 V57 G58 L59 G60
A61 A62 E63 M64 A65 T66 V67 D68 G69 W70 E71 E72 G73 G74 V75 F76 A77 W78 V79 S80 N81 T82 L83 G84 P85 F89 A90 A91 I92 S93 F94 G95 Y96 L97 Q98 I99 A100 I101 G102 F103 I104 P105 M106 F109 V110 L111 G112 A113 L114 S115 Y116 I117 L118 K119 W120 P121 A122 L123
N124 E125 D126 P127 I128 T129 K130 T131 I132 A133 I136 I137 L138 W139 A140 L141 A142 L143 T144 Q145 F146 G147 G148 T149 K150 Y151 T152 A153 R154 I155 A156 K157 V158 G159 F160 F161 A162 G163 I164 L165 L166 P167 A168 F169 I170 L171 I172 A173 L174 A175 A176 I177 Y178 L179 H180 S181 G182 A183 PRO
VAL A186 I187 E188 M189 D190 S191 K192 T193 F194 F195 P196 D197 F198 S199 K200 V201 G202 T203 L204 V205 V206 F207 V208 A209 F210 I211 L212 S213 Y214 M215 G216 V217 E218 A219 S220 A221 T222 H223 V224 M225 E226 M227 S228 N229 P230 G231 R232 D233 Y234 P235 L236 A237 M238 L239 L240 L241 M242 V243
I246 C247 L248 S249 S250 V251 G252 G253 I256 A257 M258 V259 I260 P261 G262 N263 E264 I265 N266 L267 S268 A269 G270 V271 M272 Q273 T274 F275 T276 V277 L278 M279 S280 H281 V282 A283 P284 E285 I286 T289 V290 R291 V292 I293 S294 A295 L296 L297 L298 L299 G300 V301 L302 A303 E304 I305 A306 S307
W308 I309 V310 G311 P312 S313 R314 G315 M316 Y317 V318 T319 A320 Q321 K322 N323 L324 L325 P326 F329 A330 K331 M332 N333 K334 N335 G336 V337 P338 V339 T340 L341 V342 I343 S344 Q345 L346 V347 I348 T349 S350 I351 A352 L353 I354 I355 L356 T357 N358 T359 G362 N363 N364 M365 S366 F367 L368 I369
A370 L371 A372 L373 T374 V375 V376 I377 Y378 L379 C380 A381 Y382 F383 M384 L385 F386 I387 G388 Y389 I390 V391 L392 V393 L394 K395 H396 P397 ASP LEU LYS ARG T402 F403 N404 I405 G408 K409 G410 V411 K412 L413 V414 V415 A416 I417 V418 G419 L420 L421 T422 S423 I424 M425 A426 F427 I428 V429 S430
F431 L432 P433 P434 D435 N436 I437 Q438 G439 D440 S441 T442 D443 M444 Y445 V446 E447 L448 L449 V450 V451 S452 F453 L454 V455 V456 L457 A458 L459 P460 F461 I462 L463 Y464 A465 V466 H467 ASP ARG LYS GLY LYS ALA ASN T475 G476 V477 T478 L479 E480 P481 I482 N483 S484 Q485 N486 A487 P488 K489 G490
H491 F492 F493 L494 H495 P496 R497 A498 R499 S500 P501 H502 Y503 I504 VAL MET ASN ASP LYS LYS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.62Å 105.42Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.52 – 3.19 35.52 – 3.19	Depositor EDS
% Data completeness (in resolution range)	84.2 (35.52-3.19) 84.6 (35.52-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.310 , 0.328 0.300 , 0.314	Depositor DCC
R_{free} test set	1138 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	107.4	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 87.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

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	0.77	0/3826	0.81	9/5222 (0.2%)
1	B	0.70	0/3700	0.79	5/5054 (0.1%)
All	All	0.74	0/7526	0.80	14/10276 (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
1	A	0	2

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	TYR	CB-CA-C	-8.67	93.07	110.40
1	B	215	MET	CG-SD-CE	8.39	113.62	100.20
1	B	41	SER	CB-CA-C	8.19	125.65	110.10
1	A	234	TYR	N-CA-C	7.97	132.52	111.00
1	A	482	ILE	CB-CA-C	-7.76	96.09	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ILE	Mainchain
1	A	75	VAL	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	3732	0	3867	887	0
1	B	3610	0	3738	860	0
All	All	7342	0	7605	1738	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 116.

The worst 5 of 1738 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:157:LYS:HG2	1:A:493:PHE:CD2	1.38	1.57
1:A:117:ILE:HG22	1:A:118:LEU:CD1	1.33	1.55
1:B:395:LYS:CE	1:B:396:HIS:HE1	1.18	1.53
1:A:160:PHE:CE1	1:A:165:LEU:HD23	1.46	1.51
1:A:202:GLY:CA	1:A:434:PRO:HG3	1.05	1.49

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	487/511 (95%)	374 (77%)	59 (12%)	54 (11%)	0	2
1	B	472/511 (92%)	336 (71%)	84 (18%)	52 (11%)	0	2
All	All	959/1022 (94%)	710 (74%)	143 (15%)	106 (11%)	0	2

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	86	ARG
1	A	152	THR
1	A	231	GLY
1	A	280	SER

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	394/414 (95%)	249 (63%)	145 (37%)	0 0
1	B	380/414 (92%)	234 (62%)	146 (38%)	0 0
All	All	774/828 (94%)	483 (62%)	291 (38%)	0 0

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	LEU
1	B	67	VAL
1	B	404	ASN
1	A	484	SER
1	B	15	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	GLN
1	B	266	ASN
1	B	485	GLN
1	B	124	ASN
1	B	491	HIS

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

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^{th} 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	493/511 (96%)	0.04	21 (4%)	35	21	47, 95, 150, 198	0
1	B	480/511 (93%)	0.16	30 (6%)	20	11	51, 115, 177, 251	0
All	All	973/1022 (95%)	0.10	51 (5%)	27	15	47, 105, 168, 251	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	LYS	5.2
1	B	480	GLU	4.8
1	B	435	ASP	4.5
1	B	504	ILE	3.9
1	B	196	PRO	3.9

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.