W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 08:29 AM EDT

PDB ID	:	2F1M
Title	:	Conformational flexibility in the multidrug efflux system protein AcrA
Authors	:	Mikolosko, J.; Bobyk, K.; Zgurskaya, H.I.; Ghosh, P.
Deposited on	:	2005-11-14
Resolution	:	2.71 Å(reported)

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

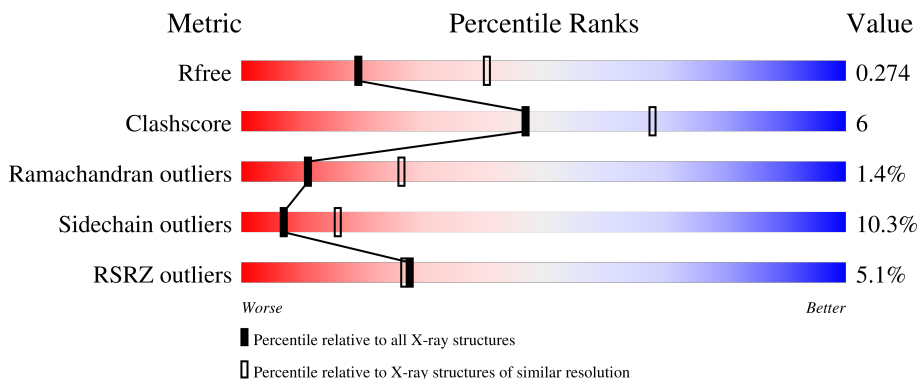|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.71 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		0.274
Clashscore		6
Ramachandran outliers		1.4%
Sidechain outliers		10.3%
RSRZ outliers		5.1%

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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	277	4% — 69% · 12% · 17%
1	B	277	4% — 63% · 15% · 19%
1	C	277	3% — 72% · 12% · · 11%
1	D	277	6% — 66% · 13% · 19%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7000 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 Acriflavine resistance protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	Se	20	0	0
			1728	1076	300	348	4			
1	B	223	Total	C	N	O	Se	25	0	0
			1680	1049	292	336	3			
1	C	247	Total	C	N	O	Se	0	0	0
			1870	1161	327	377	5			
1	D	224	Total	C	N	O	Se	21	0	0
			1686	1053	294	336	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MSE	-	initiating methionine	UNP P0AE06
A	223	MSE	PHE	engineered mutation	UNP P0AE06
A	224	MSE	LEU	engineered mutation	UNP P0AE06
A	287	MSE	LEU	engineered mutation	UNP P0AE06
A	288	MSE	LEU	engineered mutation	UNP P0AE06
A	291	MSE	MET	modified residue	UNP P0AE06
A	313	LEU	-	cloning artifact	UNP P0AE06
A	314	GLU	-	cloning artifact	UNP P0AE06
A	315	HIS	-	cloning artifact	UNP P0AE06
A	316	HIS	-	cloning artifact	UNP P0AE06
A	317	HIS	-	cloning artifact	UNP P0AE06
A	318	HIS	-	cloning artifact	UNP P0AE06
A	319	HIS	-	cloning artifact	UNP P0AE06
A	320	HIS	-	cloning artifact	UNP P0AE06
B	44	MSE	-	initiating methionine	UNP P0AE06
B	223	MSE	PHE	engineered mutation	UNP P0AE06
B	224	MSE	LEU	engineered mutation	UNP P0AE06
B	287	MSE	LEU	engineered mutation	UNP P0AE06
B	288	MSE	LEU	engineered mutation	UNP P0AE06
B	291	MSE	MET	modified residue	UNP P0AE06
B	313	LEU	-	cloning artifact	UNP P0AE06

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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
B	314	GLU	-	cloning artifact	UNP P0AE06
B	315	HIS	-	cloning artifact	UNP P0AE06
B	316	HIS	-	cloning artifact	UNP P0AE06
B	317	HIS	-	cloning artifact	UNP P0AE06
B	318	HIS	-	cloning artifact	UNP P0AE06
B	319	HIS	-	cloning artifact	UNP P0AE06
B	320	HIS	-	cloning artifact	UNP P0AE06
C	44	MSE	-	initiating methionine	UNP P0AE06
C	223	MSE	PHE	engineered mutation	UNP P0AE06
C	224	MSE	LEU	engineered mutation	UNP P0AE06
C	287	MSE	LEU	engineered mutation	UNP P0AE06
C	288	MSE	LEU	engineered mutation	UNP P0AE06
C	291	MSE	MET	modified residue	UNP P0AE06
C	313	LEU	-	cloning artifact	UNP P0AE06
C	314	GLU	-	cloning artifact	UNP P0AE06
C	315	HIS	-	cloning artifact	UNP P0AE06
C	316	HIS	-	cloning artifact	UNP P0AE06
C	317	HIS	-	cloning artifact	UNP P0AE06
C	318	HIS	-	cloning artifact	UNP P0AE06
C	319	HIS	-	cloning artifact	UNP P0AE06
C	320	HIS	-	cloning artifact	UNP P0AE06
D	44	MSE	-	initiating methionine	UNP P0AE06
D	223	MSE	PHE	engineered mutation	UNP P0AE06
D	224	MSE	LEU	engineered mutation	UNP P0AE06
D	287	MSE	LEU	engineered mutation	UNP P0AE06
D	288	MSE	LEU	engineered mutation	UNP P0AE06
D	291	MSE	MET	modified residue	UNP P0AE06
D	313	LEU	-	cloning artifact	UNP P0AE06
D	314	GLU	-	cloning artifact	UNP P0AE06
D	315	HIS	-	cloning artifact	UNP P0AE06
D	316	HIS	-	cloning artifact	UNP P0AE06
D	317	HIS	-	cloning artifact	UNP P0AE06
D	318	HIS	-	cloning artifact	UNP P0AE06
D	319	HIS	-	cloning artifact	UNP P0AE06
D	320	HIS	-	cloning artifact	UNP P0AE06

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total 14	O 14	0	0
2	B	10	Total 10	O 10	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	8	Total 8	O 8	0	0
2	D	4	Total 4	O 4	0	0

3   Residue-property plots ⓘ

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.
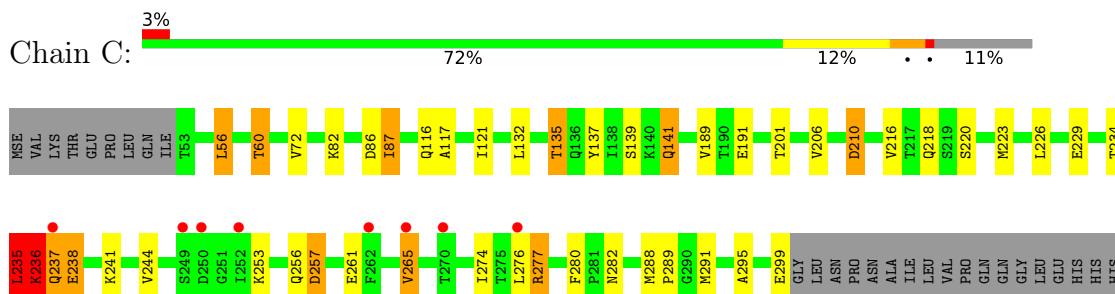
- Molecule 1: Acriflavine resistance protein A
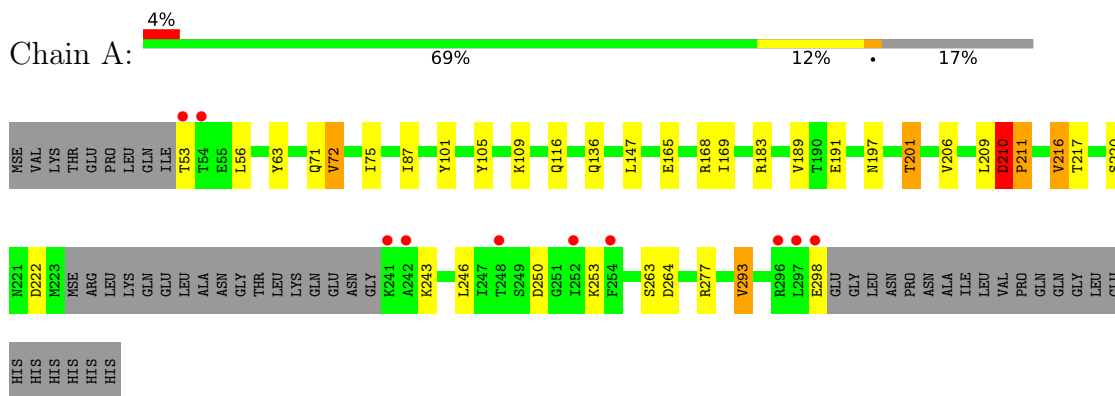
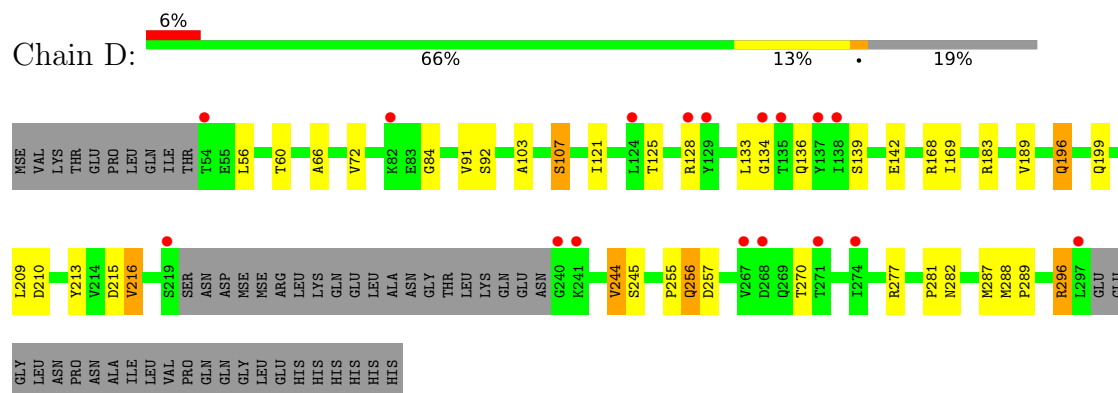- Molecule 1: Acriflavine resistance protein A
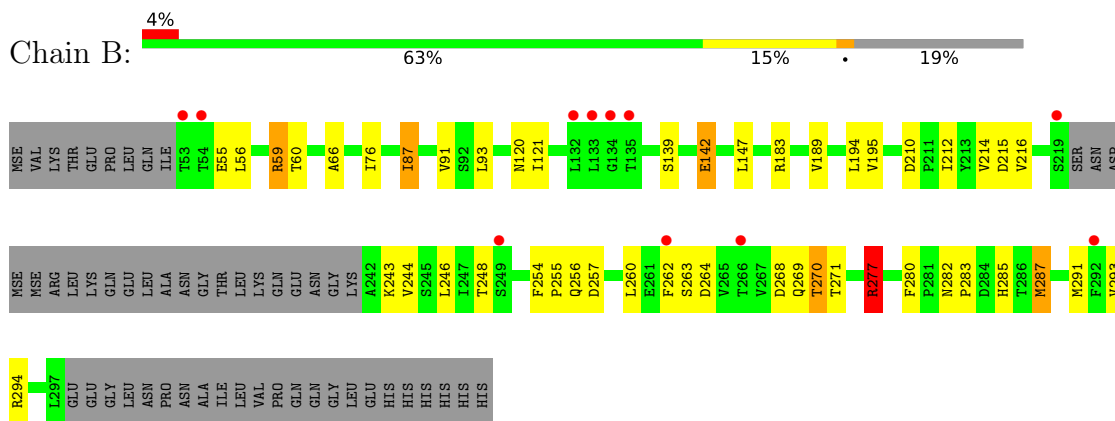
- Molecule 1: Acriflavine resistance protein A

HIS
HIS
HIS

• Molecule 1: Acriflavine resistance protein A

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	88.79Å 100.03Å 332.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.71 32.44 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-2.71) 96.7 (32.44-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.73 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.275 0.233 , 0.274	Depositor DCC
R_{free} test set	1972 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.4	EDS
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7000	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.46	0/1746	0.77	1/2364 (0.0%)
1	B	0.45	0/1699	0.80	1/2304 (0.0%)
1	C	0.45	0/1888	0.83	3/2552 (0.1%)
1	D	0.42	0/1705	0.71	0/2310
All	All	0.44	0/7038	0.78	5/9530 (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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	210	ASP	C-N-CD	6.69	142.46	128.40
1	C	277	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	277	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	222	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	257	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ASP	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	1728	0	1735	17	0
1	B	1680	0	1692	23	0
1	C	1870	0	1881	30	0
1	D	1686	0	1701	20	0
2	A	14	0	0	1	0
2	B	10	0	0	0	0
2	C	8	0	0	0	0
2	D	4	0	0	0	0
All	All	7000	0	7009	86	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 6.

The worst 5 of 86 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:91:VAL:HG22	1:D:91:VAL:HG22	1.49	0.95
1:B:277:ARG:HH11	1:B:277:ARG:HG3	1.32	0.92
1:C:236:LYS:HD2	1:C:237:GLN:H	1.37	0.88
1:C:191:GLU:O	1:D:66:ALA:HA	1.79	0.83
1:D:60:THR:HG22	1:D:289:PRO:HA	1.60	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	225/277 (81%)	213 (95%)	8 (4%)	4 (2%)	8	20
1	B	219/277 (79%)	209 (95%)	7 (3%)	3 (1%)	11	26
1	C	245/277 (88%)	236 (96%)	6 (2%)	3 (1%)	13	30
1	D	220/277 (79%)	208 (94%)	9 (4%)	3 (1%)	11	26
All	All	909/1108 (82%)	866 (95%)	30 (3%)	13 (1%)	11	26

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ASP
1	C	236	LYS
1	C	238	GLU
1	D	136	GLN
1	A	136	GLN

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	184/220 (84%)	166 (90%)	18 (10%)	8	18
1	B	178/220 (81%)	159 (89%)	19 (11%)	6	14
1	C	199/220 (90%)	173 (87%)	26 (13%)	4	9
1	D	178/220 (81%)	165 (93%)	13 (7%)	14	31
All	All	739/880 (84%)	663 (90%)	76 (10%)	7	16

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	256	GLN
1	D	216	VAL
1	C	265	VAL
1	D	107	SER
1	D	296	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	197	ASN
1	D	199	GLN
1	D	208	GLN
1	C	80	ASN
1	C	141	GLN

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 monosaccharides 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, 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	225/277 (81%)	0.14	10 (4%)	34	33	50, 62, 67, 72	5 (2%)
1	B	220/277 (79%)	0.32	11 (5%)	28	28	48, 61, 68, 74	6 (2%)
1	C	242/277 (87%)	0.27	8 (3%)	46	47	52, 61, 66, 70	0
1	D	221/277 (79%)	0.50	17 (7%)	13	12	56, 63, 69, 71	5 (2%)
All	All	908/1108 (81%)	0.31	46 (5%)	28	27	48, 61, 68, 74	16 (1%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	GLY	7.7
1	D	137	TYR	5.2
1	B	292	PHE	4.2
1	B	135	THR	4.1
1	A	298	GLU	4.0

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 monosaccharides 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.