



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:53 PM GMT

PDB ID : 3D5N
Title : Crystal structure of the Q97W15_SULSO protein from Sulfolobus solfataricus.
NESG target SsR125.
Authors : Vorobiev, S.M.; Chen, Y.; Seetharaman, J.; Lee, D.; Foote, R.E.; Maglaqui,
M.; Janjua, H.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.;
Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-05-16
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

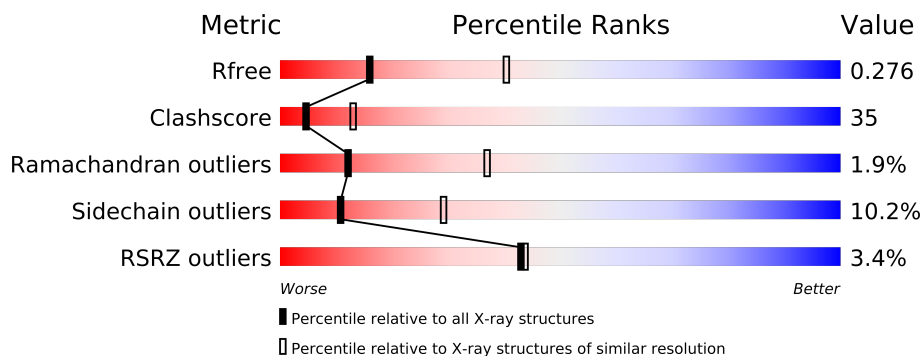
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	197	
1	B	197	
1	D	197	
1	E	197	
1	F	197	
1	G	197	
1	H	197	
1	I	197	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10496 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Q97W15_SULSO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	Se	0	0	0
			1356	882	223	243	3	5			
1	B	167	Total	C	N	O	S	Se	0	0	0
			1268	831	201	229	3	4			
1	D	178	Total	C	N	O	S	Se	0	0	0
			1373	894	226	245	3	5			
1	E	172	Total	C	N	O	S	Se	0	0	0
			1300	848	208	236	3	5			
1	F	172	Total	C	N	O	S	Se	0	0	0
			1292	847	214	223	3	5			
1	G	166	Total	C	N	O	S	Se	0	0	0
			1269	829	207	225	3	5			
1	H	173	Total	C	N	O	S	Se	0	0	0
			1315	855	212	241	3	4			
1	I	171	Total	C	N	O	S	Se	0	0	0
			1290	842	206	235	3	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	LEU	-	expression tag	UNP Q97W15
A	191	GLU	-	expression tag	UNP Q97W15
A	192	HIS	-	expression tag	UNP Q97W15
A	193	HIS	-	expression tag	UNP Q97W15
A	194	HIS	-	expression tag	UNP Q97W15
A	195	HIS	-	expression tag	UNP Q97W15
A	196	HIS	-	expression tag	UNP Q97W15
A	197	HIS	-	expression tag	UNP Q97W15
B	190	LEU	-	expression tag	UNP Q97W15
B	191	GLU	-	expression tag	UNP Q97W15
B	192	HIS	-	expression tag	UNP Q97W15
B	193	HIS	-	expression tag	UNP Q97W15
B	194	HIS	-	expression tag	UNP Q97W15

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	HIS	-	expression tag	UNP Q97W15
B	196	HIS	-	expression tag	UNP Q97W15
B	197	HIS	-	expression tag	UNP Q97W15
D	190	LEU	-	expression tag	UNP Q97W15
D	191	GLU	-	expression tag	UNP Q97W15
D	192	HIS	-	expression tag	UNP Q97W15
D	193	HIS	-	expression tag	UNP Q97W15
D	194	HIS	-	expression tag	UNP Q97W15
D	195	HIS	-	expression tag	UNP Q97W15
D	196	HIS	-	expression tag	UNP Q97W15
D	197	HIS	-	expression tag	UNP Q97W15
E	190	LEU	-	expression tag	UNP Q97W15
E	191	GLU	-	expression tag	UNP Q97W15
E	192	HIS	-	expression tag	UNP Q97W15
E	193	HIS	-	expression tag	UNP Q97W15
E	194	HIS	-	expression tag	UNP Q97W15
E	195	HIS	-	expression tag	UNP Q97W15
E	196	HIS	-	expression tag	UNP Q97W15
E	197	HIS	-	expression tag	UNP Q97W15
F	190	LEU	-	expression tag	UNP Q97W15
F	191	GLU	-	expression tag	UNP Q97W15
F	192	HIS	-	expression tag	UNP Q97W15
F	193	HIS	-	expression tag	UNP Q97W15
F	194	HIS	-	expression tag	UNP Q97W15
F	195	HIS	-	expression tag	UNP Q97W15
F	196	HIS	-	expression tag	UNP Q97W15
F	197	HIS	-	expression tag	UNP Q97W15
G	190	LEU	-	expression tag	UNP Q97W15
G	191	GLU	-	expression tag	UNP Q97W15
G	192	HIS	-	expression tag	UNP Q97W15
G	193	HIS	-	expression tag	UNP Q97W15
G	194	HIS	-	expression tag	UNP Q97W15
G	195	HIS	-	expression tag	UNP Q97W15
G	196	HIS	-	expression tag	UNP Q97W15
G	197	HIS	-	expression tag	UNP Q97W15
H	190	LEU	-	expression tag	UNP Q97W15
H	191	GLU	-	expression tag	UNP Q97W15
H	192	HIS	-	expression tag	UNP Q97W15
H	193	HIS	-	expression tag	UNP Q97W15
H	194	HIS	-	expression tag	UNP Q97W15
H	195	HIS	-	expression tag	UNP Q97W15
H	196	HIS	-	expression tag	UNP Q97W15

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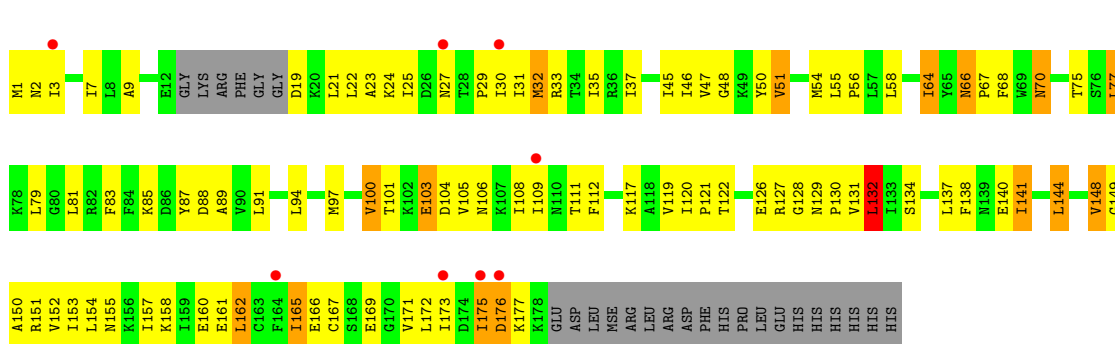
Chain	Residue	Modelled	Actual	Comment	Reference
H	197	HIS	-	expression tag	UNP Q97W15
I	190	LEU	-	expression tag	UNP Q97W15
I	191	GLU	-	expression tag	UNP Q97W15
I	192	HIS	-	expression tag	UNP Q97W15
I	193	HIS	-	expression tag	UNP Q97W15
I	194	HIS	-	expression tag	UNP Q97W15
I	195	HIS	-	expression tag	UNP Q97W15
I	196	HIS	-	expression tag	UNP Q97W15
I	197	HIS	-	expression tag	UNP Q97W15

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	4	Total O 4 4	0	0
2	D	6	Total O 6 6	0	0
2	E	4	Total O 4 4	0	0
2	F	4	Total O 4 4	0	0
2	G	2	Total O 2 2	0	0
2	H	5	Total O 5 5	0	0
2	I	5	Total O 5 5	0	0

- Molecule 1: Q97W15_SULSO

Chain E:



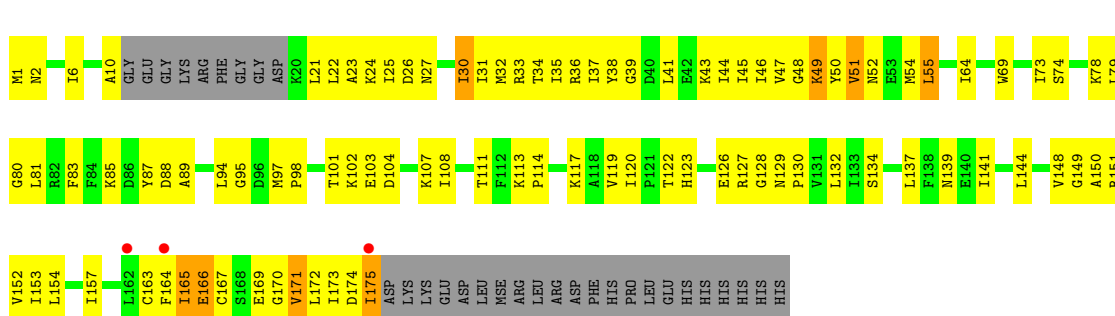
- Molecule 1: Q97W15_SULSO

Chain F:



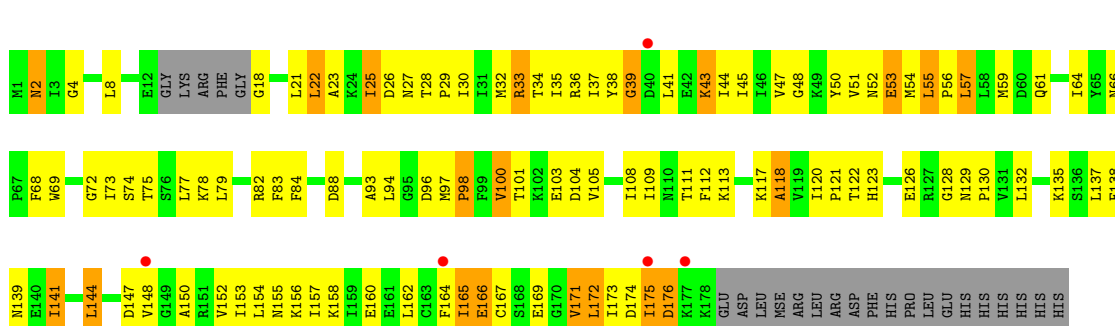
- Molecule 1: Q97W15_SULSO

Chain G:

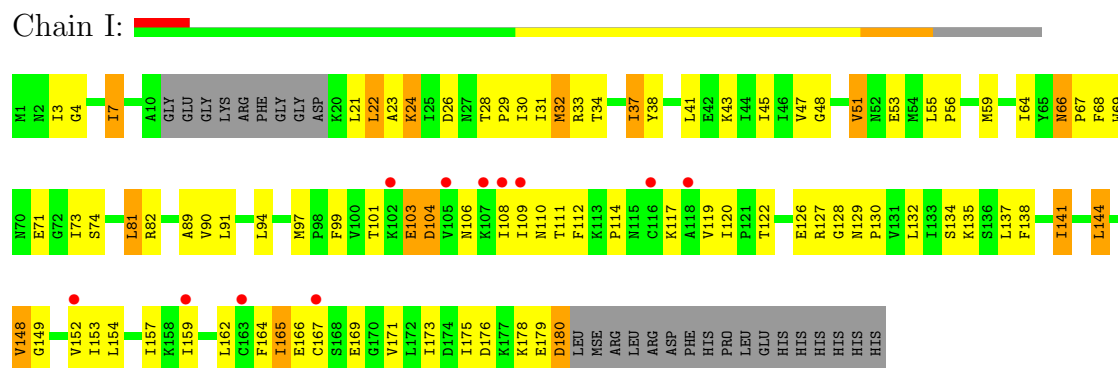


- Molecule 1: Q97W15_SULSO

Chain H:



Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.96Å 169.23Å 173.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.80 48.47 – 2.77	Depositor EDS
% Data completeness (in resolution range)	86.2 (48.47-2.80) 96.7 (48.47-2.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.266 0.244 , 0.276	Depositor DCC
R_{free} test set	3140 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.1	EDS
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 126312 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10496	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0/1373	0.70	0/1852
1	B	0.41	0/1283	0.71	1/1734 (0.1%)
1	D	0.40	0/1390	0.69	0/1870
1	E	0.45	0/1315	0.70	1/1778 (0.1%)
1	F	0.41	0/1307	0.68	0/1765
1	G	0.41	0/1284	0.71	0/1736
1	H	0.48	0/1330	0.70	0/1797
1	I	0.38	0/1305	0.68	0/1767
All	All	0.42	0/10587	0.70	2/14299 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	132	LEU	CA-CB-CG	5.60	128.19	115.30
1	B	144	LEU	CA-CB-CG	5.57	128.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1356	0	1391	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1268	0	1300	76	0
1	D	1373	0	1430	91	0
1	E	1300	0	1324	105	0
1	F	1292	0	1335	96	0
1	G	1269	0	1309	98	0
1	H	1315	0	1339	122	0
1	I	1290	0	1305	110	0
2	A	3	0	0	0	0
2	B	4	0	0	1	0
2	D	6	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	2	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
All	All	10496	0	10733	740	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

The worst 5 of 740 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:111:THR:HG21	1:G:165:ILE:HG21	1.20	1.10
1:A:18:GLY:HA3	1:A:50:TYR:HB2	1.31	1.09
1:H:66:ASN:HD21	1:H:75:THR:HG23	1.17	1.09
1:E:68:PHE:HB2	1:E:75:THR:HG21	1.34	1.08
1:G:81:LEU:HD22	1:G:141:ILE:HD11	1.37	1.06

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	176/197 (89%)	155 (88%)	18 (10%)	3 (2%)	14 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/197 (83%)	141 (86%)	19 (12%)	3 (2%)	13	39
1	D	176/197 (89%)	157 (89%)	18 (10%)	1 (1%)	33	72
1	E	168/197 (85%)	150 (89%)	14 (8%)	4 (2%)	9	29
1	F	168/197 (85%)	152 (90%)	16 (10%)	0	100	100
1	G	162/197 (82%)	142 (88%)	15 (9%)	5 (3%)	7	21
1	H	169/197 (86%)	149 (88%)	14 (8%)	6 (4%)	5	17
1	I	167/197 (85%)	147 (88%)	17 (10%)	3 (2%)	13	39
All	All	1349/1576 (86%)	1193 (88%)	131 (10%)	25 (2%)	12	37

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	85	LYS
1	B	171	VAL
1	D	159	ILE
1	G	49	LYS
1	H	155	ASN

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	144/169 (85%)	128 (89%)	16 (11%)	9	25
1	B	136/169 (80%)	120 (88%)	16 (12%)	8	22
1	D	148/169 (88%)	132 (89%)	16 (11%)	9	26
1	E	139/169 (82%)	123 (88%)	16 (12%)	8	23
1	F	135/169 (80%)	125 (93%)	10 (7%)	20	48
1	G	137/169 (81%)	128 (93%)	9 (7%)	24	56
1	H	141/169 (83%)	125 (89%)	16 (11%)	9	24
1	I	137/169 (81%)	122 (89%)	15 (11%)	9	26
All	All	1117/1352 (83%)	1003 (90%)	114 (10%)	11	29

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	66	ASN
1	E	176	ASP
1	I	66	ASN
1	E	77	LEU
1	E	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	66	ASN
1	E	2	ASN
1	H	110	ASN
1	D	106	ASN
1	D	155	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	178/197 (90%)	0.22	4 (2%) 59 60	42, 66, 92, 98	0
1	B	167/197 (84%)	0.41	7 (4%) 35 35	39, 70, 99, 100	0
1	D	178/197 (90%)	0.32	4 (2%) 59 60	45, 69, 95, 100	0
1	E	172/197 (87%)	0.36	8 (4%) 30 30	28, 69, 89, 98	0
1	F	172/197 (87%)	0.34	5 (2%) 49 50	34, 74, 100, 100	0
1	G	166/197 (84%)	0.29	3 (1%) 65 66	45, 71, 91, 97	0
1	H	173/197 (87%)	0.28	5 (2%) 49 50	33, 68, 93, 95	0
1	I	171/197 (86%)	0.48	11 (6%) 19 17	44, 77, 100, 100	0
All	All	1377/1576 (87%)	0.34	47 (3%) 43 44	28, 71, 97, 100	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	108	ILE	5.5
1	A	18	GLY	5.3
1	B	175	ILE	5.1
1	A	17	GLY	4.8
1	E	175	ILE	4.3

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.