wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 06:45 PM EDT

PDB ID	:	5NT2
Title	:	Complex of influenza A NS1 with TRIM25 coiled coil domain
Authors	:	Koliopoulos, M.G.; Rittinger, K.
Deposited on	:	2017-04-27
Resolution	:	4.26 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:

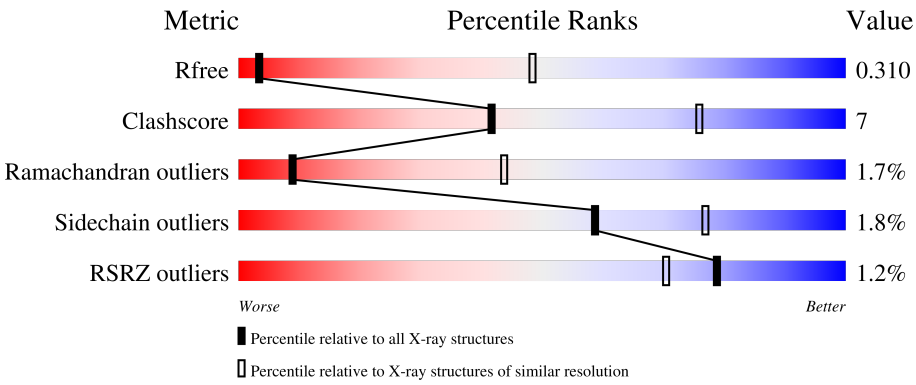
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 4.26 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	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)
RSRZ outliers	127900	1072 (4.80-3.70)

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	C	233	41% 8% 51%
1	D	233	69% 16% • 14%
1	E	233	% 65% 18% • 14%
1	F	233	43% 6% 51%
2	A	193	74% 15% • 10%

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Mol	Chain	Length	Quality of chain
2	I	193	% 68% 20% •• 10%
2	N	193	4% 75% 13% • 10%
2	V	193	2% 73% 16% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10516 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	115	894	567	152	169	6	0	0	0
1	C	115	895	567	152	170	6	0	0	0
1	D	200	1559	979	274	297	9	0	0	0
1	E	201	1566	984	275	298	9	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P03496
F	-1	PRO	-	expression tag	UNP P03496
F	0	GLY	-	expression tag	UNP P03496
F	38	ALA	ARG	engineered mutation	UNP P03496
F	41	ALA	LYS	engineered mutation	UNP P03496
F	101	GLU	ASP	variant	UNP P03496
F	187	ALA	TRP	engineered mutation	UNP P03496
C	-2	GLY	-	expression tag	UNP P03496
C	-1	PRO	-	expression tag	UNP P03496
C	0	GLY	-	expression tag	UNP P03496
C	38	ALA	ARG	engineered mutation	UNP P03496
C	41	ALA	LYS	engineered mutation	UNP P03496
C	101	GLU	ASP	variant	UNP P03496
C	187	ALA	TRP	engineered mutation	UNP P03496
D	-2	GLY	-	expression tag	UNP P03496
D	-1	PRO	-	expression tag	UNP P03496
D	0	GLY	-	expression tag	UNP P03496
D	38	ALA	ARG	engineered mutation	UNP P03496
D	41	ALA	LYS	engineered mutation	UNP P03496
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P03496
E	-1	PRO	-	expression tag	UNP P03496
E	0	GLY	-	expression tag	UNP P03496
E	38	ALA	ARG	engineered mutation	UNP P03496
E	41	ALA	LYS	engineered mutation	UNP P03496
E	101	GLU	ASP	variant	UNP P03496
E	187	ALA	TRP	engineered mutation	UNP P03496

- Molecule 2 is a protein called E3 ubiquitin/ISG15 ligase TRIM25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	173	1399	868	250	277	4	0	0	0
			Total	C	N	O	S			
2	A	173	1401	869	250	278	4	0	0	0
			Total	C	N	O	S			
2	V	173	1401	869	250	278	4	0	0	0
			Total	C	N	O	S			
2	N	173	1401	869	250	278	4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

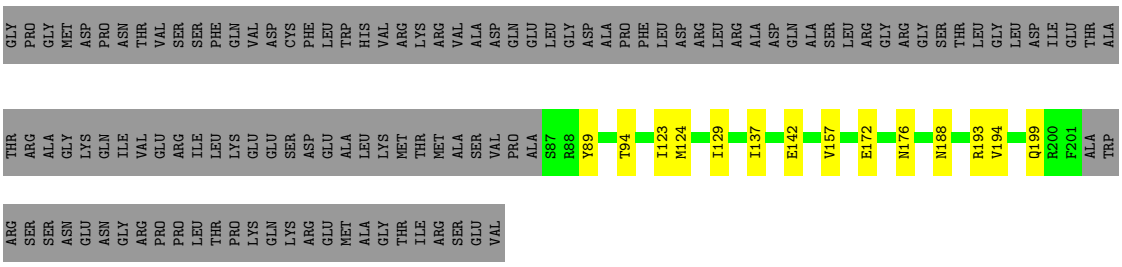
Chain	Residue	Modelled	Actual	Comment	Reference
I	187	GLY	-	expression tag	UNP Q14258
I	188	PRO	-	expression tag	UNP Q14258
I	189	GLY	-	expression tag	UNP Q14258
I	358	LEU	PRO	variant	UNP Q14258
A	187	GLY	-	expression tag	UNP Q14258
A	188	PRO	-	expression tag	UNP Q14258
A	189	GLY	-	expression tag	UNP Q14258
A	358	LEU	PRO	variant	UNP Q14258
V	187	GLY	-	expression tag	UNP Q14258
V	188	PRO	-	expression tag	UNP Q14258
V	189	GLY	-	expression tag	UNP Q14258
V	358	LEU	PRO	variant	UNP Q14258
N	187	GLY	-	expression tag	UNP Q14258
N	188	PRO	-	expression tag	UNP Q14258
N	189	GLY	-	expression tag	UNP Q14258
N	358	LEU	PRO	variant	UNP Q14258

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.

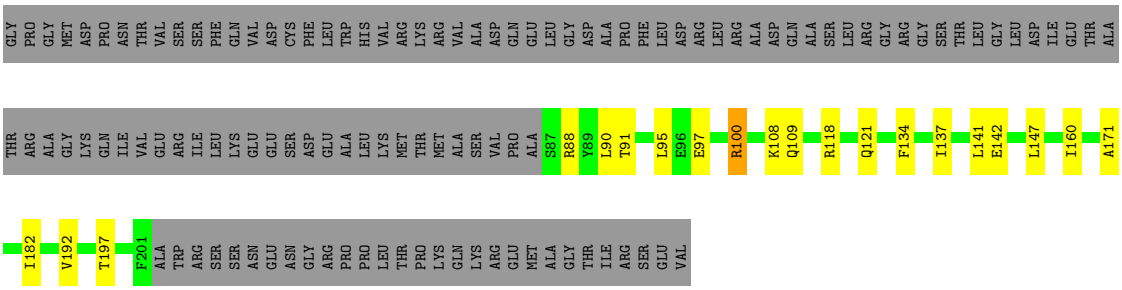
• Molecule 1: Non-structural protein 1

Chain F:



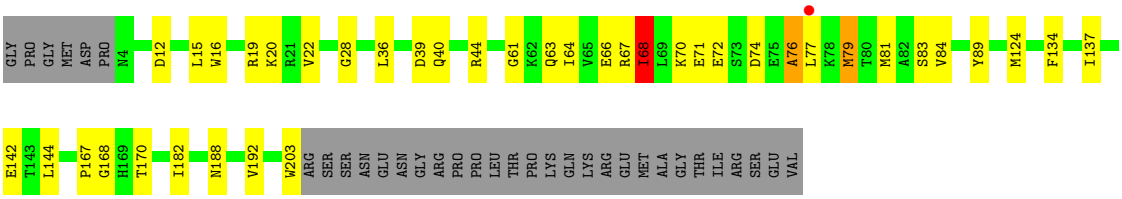
• Molecule 1: Non-structural protein 1

Chain C:



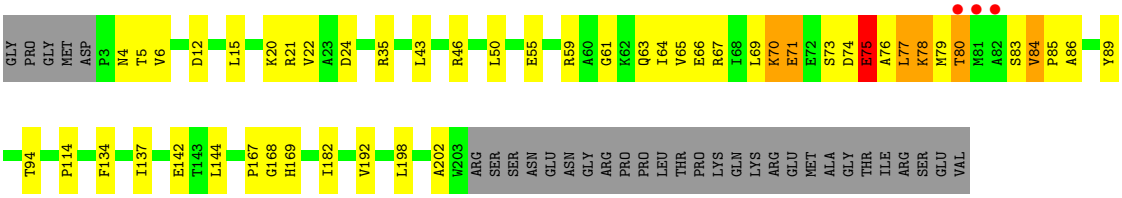
• Molecule 1: Non-structural protein 1

Chain D:



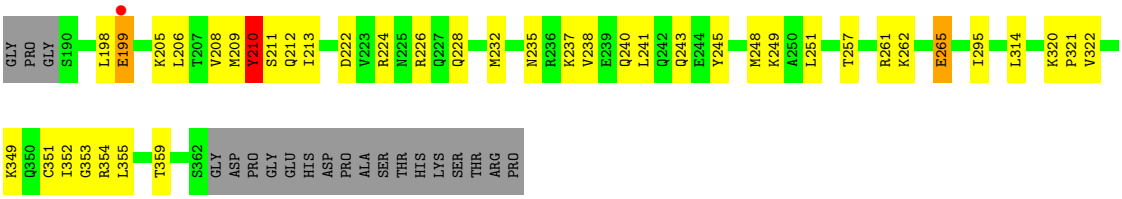
• Molecule 1: Non-structural protein 1

Chain E:



- Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25

Chain I:

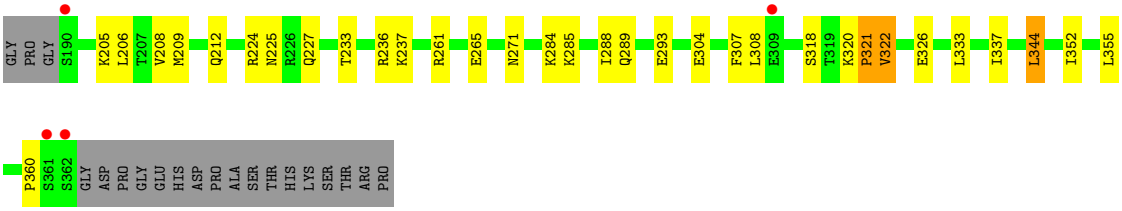


- Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25

Chain A:

- Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25

Chain V:



- Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.26Å 76.30Å 92.07Å 100.04° 93.71° 111.14°	Depositor
Resolution (Å)	61.68 – 4.26 61.68 – 4.26	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.68-4.26) 98.0 (61.68-4.26)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.270 , 0.309 0.270 , 0.310	Depositor DCC
R_{free} test set	635 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	122.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 110.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10516	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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	C	0.25	0/907	0.51	0/1226
1	D	0.26	0/1581	0.50	0/2136
1	E	0.27	0/1589	0.52	1/2147 (0.0%)
1	F	0.25	0/906	0.49	0/1224
2	A	0.29	0/1413	0.50	0/1892
2	I	0.30	0/1411	0.55	1/1889 (0.1%)
2	N	0.29	0/1413	0.50	0/1892
2	V	0.29	0/1413	0.49	0/1892
All	All	0.28	0/10633	0.51	2/14298 (0.0%)

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	E	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	84	VAL	C-N-CD	-6.33	106.68	120.60
2	I	210	TYR	CA-CB-CG	6.06	124.92	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	71	GLU	Peptide
1	E	73	SER	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	C	895	0	921	11	0
1	D	1559	0	1586	28	0
1	E	1566	0	1594	34	0
1	F	894	0	921	8	0
2	A	1401	0	1450	24	0
2	I	1399	0	1446	30	0
2	N	1401	0	1450	26	0
2	V	1401	0	1450	26	0
All	All	10516	0	10818	149	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 7.

The worst 5 of 149 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)
2:I:261:ARG:NH2	2:N:361:SER:OG	2.17	0.77
1:D:68:ILE:HA	1:D:70:LYS:H	1.52	0.74
2:I:224:ARG:NH2	2:N:278:TYR:OH	2.23	0.72
2:N:315:ARG:HG3	2:N:316:GLY:H	1.56	0.70
1:D:19:ARG:NH1	1:D:39:ASP:OD2	2.24	0.69

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	C	113/233 (48%)	112 (99%)	1 (1%)	0	100	100
1	D	198/233 (85%)	174 (88%)	19 (10%)	5 (2%)	5	35
1	E	199/233 (85%)	174 (87%)	18 (9%)	7 (4%)	3	29
1	F	113/233 (48%)	112 (99%)	1 (1%)	0	100	100
2	A	171/193 (89%)	166 (97%)	3 (2%)	2 (1%)	13	50
2	I	171/193 (89%)	165 (96%)	4 (2%)	2 (1%)	13	50
2	N	171/193 (89%)	164 (96%)	3 (2%)	4 (2%)	6	37
2	V	171/193 (89%)	166 (97%)	3 (2%)	2 (1%)	13	50
All	All	1307/1704 (77%)	1233 (94%)	52 (4%)	22 (2%)	9	44

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	78	LYS
1	E	85	PRO
2	I	321	PRO
2	A	321	PRO
2	V	321	PRO

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	C	100/198 (50%)	97 (97%)	3 (3%)	41	63
1	D	170/198 (86%)	167 (98%)	3 (2%)	59	77
1	E	171/198 (86%)	165 (96%)	6 (4%)	36	60
1	F	100/198 (50%)	100 (100%)	0	100	100
2	A	160/175 (91%)	160 (100%)	0	100	100
2	I	159/175 (91%)	155 (98%)	4 (2%)	47	68
2	N	160/175 (91%)	157 (98%)	3 (2%)	57	75
2	V	160/175 (91%)	158 (99%)	2 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1180/1492 (79%)	1159 (98%)	21 (2%)	59 77

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	257	THR
2	V	344	LEU
2	N	344	LEU
2	N	261	ARG
2	V	293	GLU

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

Mol	Chain	Res	Type
2	A	271	ASN
2	V	227	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	C	115/233 (49%)	-0.12	0	100	100	112, 139, 177, 203	0
1	D	200/233 (85%)	-0.15	1 (0%)	91	86	115, 169, 241, 260	0
1	E	201/233 (86%)	-0.12	3 (1%)	73	64	113, 154, 208, 240	0
1	F	115/233 (49%)	-0.19	0	100	100	112, 140, 178, 196	0
2	A	173/193 (89%)	-0.08	0	100	100	112, 141, 241, 259	0
2	I	173/193 (89%)	-0.08	1 (0%)	89	84	118, 147, 252, 284	0
2	N	173/193 (89%)	-0.01	7 (4%)	38	30	109, 147, 327, 404	0
2	V	173/193 (89%)	-0.05	4 (2%)	60	51	111, 148, 260, 285	0
All	All	1323/1704 (77%)	-0.10	16 (1%)	79	70	109, 149, 241, 404	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	362	SER	5.9
2	N	314	LEU	3.7
2	V	190	SER	3.6
2	N	311	ALA	3.1
1	E	81	MET	2.8

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.