



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:33 PM GMT

PDB ID : 4CKN
Title : Structure of an N-terminal fragment of Leishmania SAS-6 containing parts of its coiled coil domain, F257E mutant
Authors : van Breugel, M.
Deposited on : 2014-01-07
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

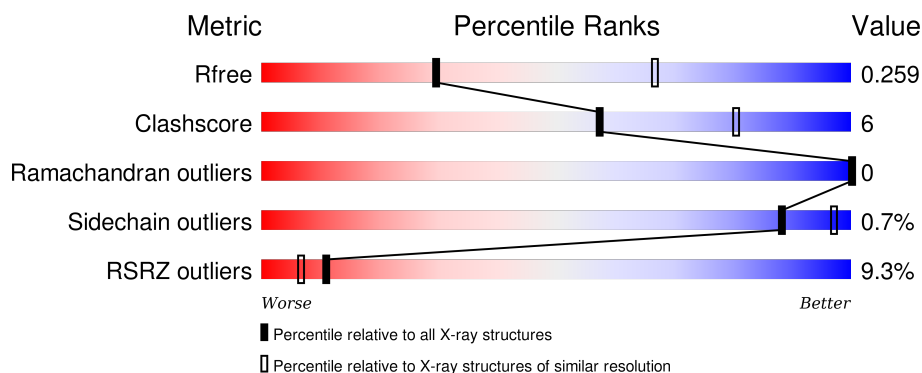
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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 $\leq 5\%$. 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	226	<div> <div>10%</div> <div>69%</div> <div>10%</div> <div>21%</div> </div>
1	B	226	<div> <div>10%</div> <div>71%</div> <div>8%</div> <div>20%</div> </div>
1	C	226	<div> <div>2%</div> <div>68%</div> <div>12%</div> <div>20%</div> </div>
1	D	226	<div> <div>7%</div> <div>66%</div> <div>10%</div> <div>24%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5653 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 SAS-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1417	900	247	267	3			
1	B	180	Total	C	N	O	S	0	0	0
			1432	908	249	272	3			
1	C	181	Total	C	N	O	S	0	0	0
			1440	912	251	274	3			
1	D	172	Total	C	N	O	S	0	0	0
			1364	864	238	259	3			

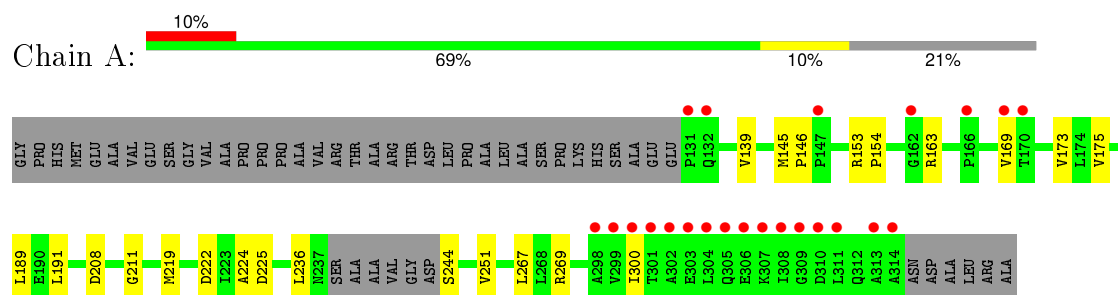
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
A	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
A	257	GLU	PHE	ENGINEERED MUTATION	UNP E9AFQ5
B	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
B	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
B	257	GLU	PHE	ENGINEERED MUTATION	UNP E9AFQ5
C	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
C	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
C	257	GLU	PHE	ENGINEERED MUTATION	UNP E9AFQ5
D	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
D	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
D	257	GLU	PHE	ENGINEERED MUTATION	UNP E9AFQ5

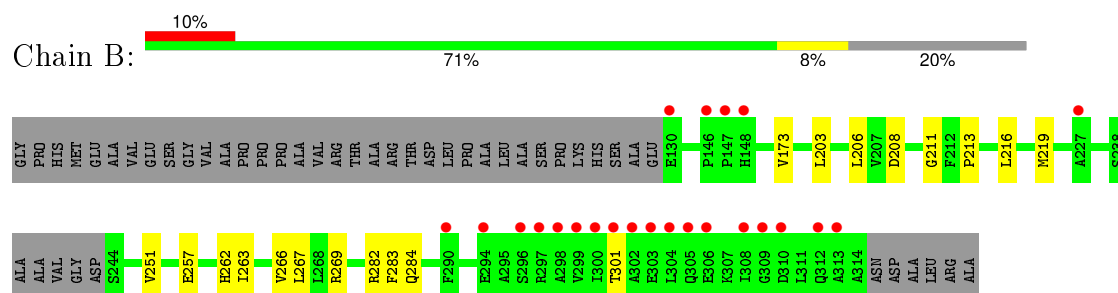
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

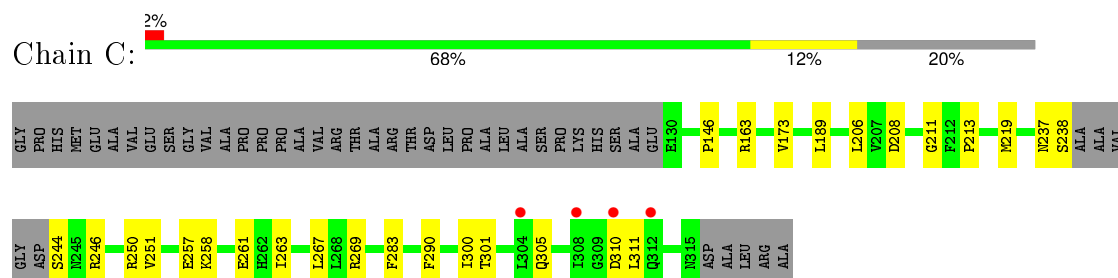
• Molecule 1: SAS-6



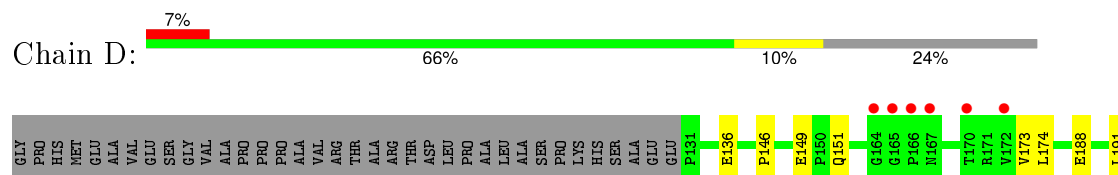
• Molecule 1: SAS-6

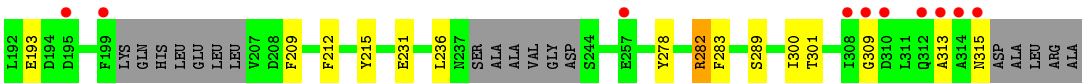


• Molecule 1: SAS-6



• Molecule 1: SAS-6





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.86Å 81.25Å 133.15Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	133.10 – 2.90 46.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (133.10-2.90) 97.8 (46.91-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0047	Depositor
R, R_{free}	0.237 , 0.256 0.238 , 0.259	Depositor DCC
R_{free} test set	1279 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	80.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25370 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5653	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/1444	0.63	0/1956
1	B	0.40	0/1459	0.68	2/1977 (0.1%)
1	C	0.43	0/1467	0.70	0/1988
1	D	0.47	0/1389	0.79	2/1881 (0.1%)
All	All	0.43	0/5759	0.70	4/7802 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	D	282	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	B	269	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	282	ARG	NE-CZ-NH1	5.53	123.06	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1417	0	1414	18	0
1	B	1432	0	1424	16	1
1	C	1440	0	1430	22	1
1	D	1364	0	1352	19	0
All	All	5653	0	5620	68	1

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.

All (68) 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:D:136:GLU:OE2	1:D:282:ARG:NH2	2.10	0.85
1:D:309:GLY:O	1:D:313:ALA:CB	2.26	0.84
1:D:309:GLY:O	1:D:313:ALA:HB2	1.78	0.82
1:A:146:PRO:HD2	1:A:236:LEU:HD12	1.67	0.76
1:C:219:MET:CE	1:C:251:VAL:HG11	2.15	0.75
1:A:175:VAL:HG22	1:A:189:LEU:HB3	1.74	0.68
1:C:310:ASP:OD1	1:C:311:LEU:N	2.26	0.67
1:C:250:ARG:NH1	1:C:261:GLU:OE1	2.29	0.66
1:D:174:LEU:HD11	1:D:188:GLU:HG3	1.78	0.65
1:D:309:GLY:O	1:D:313:ALA:HB3	1.98	0.63
1:A:219:MET:CE	1:A:251:VAL:HG11	2.28	0.63
1:C:219:MET:HE1	1:C:251:VAL:HG11	1.80	0.63
1:A:163:ARG:HD2	1:A:169:VAL:O	2.00	0.61
1:C:300:ILE:HG21	1:D:301:THR:HG22	1.82	0.61
1:C:219:MET:HE2	1:C:251:VAL:HG11	1.83	0.61
1:D:193:GLU:HA	1:D:209:PHE:CE1	2.36	0.60
1:B:206:LEU:N	1:C:257:GLU:O	2.28	0.58
1:A:219:MET:HE2	1:A:251:VAL:HG11	1.85	0.58
1:B:257:GLU:O	1:C:206:LEU:N	2.33	0.56
1:C:301:THR:HG22	1:D:300:ILE:HG21	1.87	0.56
1:A:139:VAL:HG22	1:A:224:ALA:HB2	1.85	0.56
1:C:251:VAL:HB	1:C:263:ILE:HG22	1.89	0.55
1:D:174:LEU:CD1	1:D:188:GLU:HG3	2.36	0.54
1:B:251:VAL:HB	1:B:263:ILE:HG12	1.92	0.52
1:D:173:VAL:HG13	1:D:191:LEU:HB3	1.93	0.51
1:B:267:LEU:N	1:B:267:LEU:HD12	2.27	0.50
1:A:173:VAL:HG13	1:A:191:LEU:HB3	1.94	0.49
1:C:237:ASN:OD1	1:C:244:SER:HA	2.12	0.49
1:A:300:ILE:HG21	1:B:301:THR:HG22	1.95	0.48
1:A:219:MET:HE1	1:A:251:VAL:HG11	1.94	0.48
1:A:153:ARG:HG3	1:A:154:PRO:HD2	1.96	0.48
1:B:267:LEU:N	1:B:267:LEU:CD1	2.77	0.48
1:C:290:PHE:CE1	1:D:289:SER:HB3	2.48	0.47
1:B:173:VAL:HG21	1:B:213:PRO:HG3	1.96	0.47
1:B:251:VAL:CG2	1:B:263:ILE:HD11	2.45	0.47
1:D:278:TYR:CE1	1:D:282:ARG:HG2	2.50	0.47
1:C:173:VAL:HG21	1:C:213:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HD13	1:B:263:ILE:HD12	1.97	0.46
1:B:262:HIS:O	1:B:263:ILE:HG23	2.16	0.46
1:D:146:PRO:HD2	1:D:236:LEU:HD23	1.97	0.46
1:C:301:THR:O	1:C:305:GLN:HB2	2.14	0.46
1:A:145:MET:HA	1:A:236:LEU:HD12	1.98	0.46
1:B:266:VAL:C	1:B:267:LEU:HD12	2.37	0.45
1:B:219:MET:CE	1:B:263:ILE:HD13	2.47	0.45
1:A:153:ARG:CG	1:A:154:PRO:HD2	2.47	0.45
1:A:244:SER:O	1:A:269:ARG:NH1	2.49	0.45
1:A:146:PRO:CD	1:A:236:LEU:HD12	2.44	0.44
1:B:251:VAL:HG23	1:B:263:ILE:HD11	1.99	0.44
1:D:315:ASN:C	1:D:315:ASN:OD1	2.55	0.44
1:D:278:TYR:CE1	1:D:282:ARG:CG	3.01	0.44
1:B:208:ASP:HB2	1:B:211:GLY:H	1.82	0.43
1:D:282:ARG:HD2	1:D:282:ARG:HA	1.69	0.43
1:A:208:ASP:HB2	1:A:211:GLY:H	1.83	0.43
1:D:149:GLU:O	1:D:151:GLN:HB2	2.18	0.43
1:C:208:ASP:HB2	1:C:211:GLY:H	1.83	0.43
1:C:219:MET:HE1	1:C:251:VAL:CG1	2.48	0.43
1:C:189:LEU:HB2	1:C:267:LEU:HD23	2.01	0.43
1:B:216:LEU:HD13	1:B:263:ILE:CD1	2.49	0.42
1:A:222:ASP:O	1:A:225:ASP:OD1	2.37	0.42
1:C:146:PRO:HG3	1:C:238:SER:CB	2.49	0.42
1:C:237:ASN:ND2	1:C:246:ARG:HG2	2.34	0.42
1:A:173:VAL:CG1	1:A:191:LEU:HB3	2.50	0.41
1:D:173:VAL:CG1	1:D:191:LEU:HB3	2.50	0.41
1:C:244:SER:O	1:C:269:ARG:NH1	2.54	0.41
1:B:203:LEU:O	1:C:258:LYS:HE3	2.21	0.41
1:C:146:PRO:HG3	1:C:238:SER:HB2	2.03	0.41
1:A:189:LEU:HB2	1:A:267:LEU:HD23	2.02	0.41
1:D:212:PHE:O	1:D:215:TYR:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLN:OE1	1:C:163:ARG:NH1[3_555]	2.08	0.12

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	174/226 (77%)	173 (99%)	1 (1%)	0	100	100
1	B	176/226 (78%)	174 (99%)	2 (1%)	0	100	100
1	C	177/226 (78%)	174 (98%)	3 (2%)	0	100	100
1	D	166/226 (74%)	164 (99%)	2 (1%)	0	100	100
All	All	693/904 (77%)	685 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	154/188 (82%)	154 (100%)	0	100	100
1	B	156/188 (83%)	155 (99%)	1 (1%)	90	97
1	C	157/188 (84%)	156 (99%)	1 (1%)	90	97
1	D	148/188 (79%)	146 (99%)	2 (1%)	74	93
All	All	615/752 (82%)	611 (99%)	4 (1%)	88	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	283	PHE
1	C	283	PHE

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Mol	Chain	Res	Type
1	D	231	GLU
1	D	283	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	B	197	ASN
1	B	202	HIS
1	C	284	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 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 ⓘ

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	178/226 (78%)	0.85	23 (12%) 5 3	66, 110, 165, 195	0
1	B	180/226 (79%)	0.70	23 (12%) 5 3	57, 80, 162, 197	0
1	C	181/226 (80%)	0.43	4 (2%) 65 60	49, 73, 138, 173	0
1	D	172/226 (76%)	0.71	16 (9%) 11 7	60, 84, 143, 171	0
All	All	711/904 (78%)	0.67	66 (9%) 11 7	49, 85, 158, 197	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	GLY	7.6
1	A	305	GLN	6.3
1	A	302	ALA	5.6
1	A	314	ALA	5.2
1	A	309	GLY	5.2
1	A	311	LEU	5.0
1	C	312	GLN	5.0
1	A	310	ASP	4.9
1	A	301	THR	4.6
1	D	167	ASN	4.5
1	A	300	ILE	4.5
1	B	300	ILE	4.5
1	B	304	LEU	4.2
1	B	313	ALA	4.2
1	A	304	LEU	4.1
1	D	312	GLN	4.1
1	B	303	GLU	3.8
1	D	166	PRO	3.8
1	A	308	ILE	3.7
1	A	303	GLU	3.6
1	D	165	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	310	ASP	3.5
1	A	307	LYS	3.3
1	D	313	ALA	3.2
1	B	301	THR	3.2
1	B	148	HIS	3.1
1	A	313	ALA	3.0
1	D	195	ASP	3.0
1	D	314	ALA	3.0
1	A	306	GLU	3.0
1	A	166	PRO	3.0
1	D	309	GLY	3.0
1	B	147	PRO	2.9
1	B	312	GLN	2.9
1	A	170	THR	2.8
1	B	290	PHE	2.8
1	A	147	PRO	2.8
1	D	170	THR	2.7
1	B	302	ALA	2.7
1	B	130	GLU	2.7
1	C	304	LEU	2.6
1	D	199	PHE	2.6
1	A	162	GLY	2.6
1	D	172	VAL	2.6
1	A	132	GLN	2.5
1	C	310	ASP	2.5
1	B	299	VAL	2.4
1	D	315	ASN	2.4
1	B	296	SER	2.3
1	C	308	ILE	2.3
1	B	146	PRO	2.3
1	A	298	ALA	2.3
1	B	297	ARG	2.3
1	B	294	GLU	2.2
1	B	308	ILE	2.2
1	B	306	GLU	2.2
1	D	310	ASP	2.1
1	A	169	VAL	2.1
1	B	298	ALA	2.1
1	D	164	GLY	2.1
1	B	305	GLN	2.1
1	A	131	PRO	2.1
1	A	299	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	2.1
1	D	257	GLU	2.0
1	D	308	ILE	2.0

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.