



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:24 pm GMT

PDB ID : 2V3C
Title : CRYSTAL STRUCTURE OF THE SRP54-SRP19-7S.S SRP RNA COMPLEX OF M. JANNASCHII
Authors : Hainzl, T.; Huang, S.; Sauer-Eriksson, A.E.
Deposited on : 2007-06-15
Resolution : 2.50 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

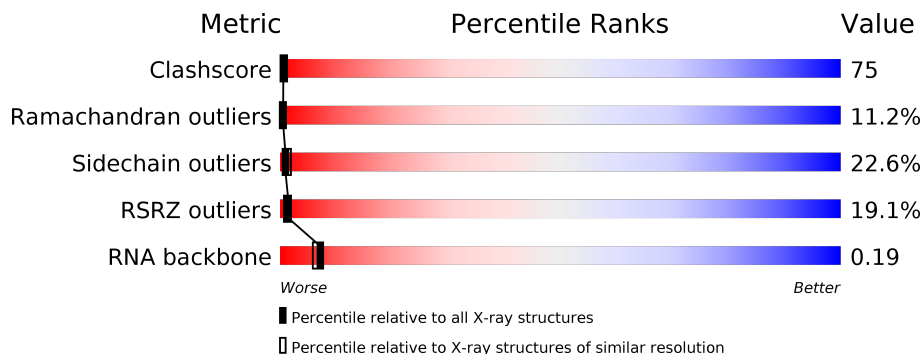
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)
RNA backbone	2435	1019 (2.90-2.10)

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	87	<div> <div>34%</div> <div>51%</div> <div>14%</div> <div>.</div> </div>
1	B	87	<div> <div>30%</div> <div>45%</div> <div>25%</div> </div>
2	C	432	<div> <div>17%</div> <div>20%</div> <div>50%</div> <div>19%</div> <div>5%</div> <div>6%</div> </div>
2	D	432	<div> <div>34%</div> <div>13%</div> <div>53%</div> <div>23%</div> <div>7%</div> </div>
3	M	96	<div> <div>17%</div> <div>44%</div> <div>40%</div> </div>
3	N	96	<div> <div>23%</div> <div>47%</div> <div>30%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12336 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 SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	0	0	0
			727	468	130	125	4			
1	B	87	Total	C	N	O	S	0	0	0
			727	468	130	125	4			

- Molecule 2 is a protein called SIGNAL RECOGNITION 54 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	404	Total	C	N	O	S	0	0	1
			3149	1998	541	600	10			
2	D	402	Total	C	N	O	S	0	0	1
			3133	1989	538	597	9			

- Molecule 3 is a RNA chain called 7S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	96	Total	C	N	O	P	0	0	0
			2063	919	385	664	95			
3	N	96	Total	C	N	O	P	0	0	0
			2063	919	385	664	95			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	26	Total	O	0	0
			26	26		
4	C	107	Total	O	0	0
			107	107		
4	D	107	Total	O	0	0
			107	107		

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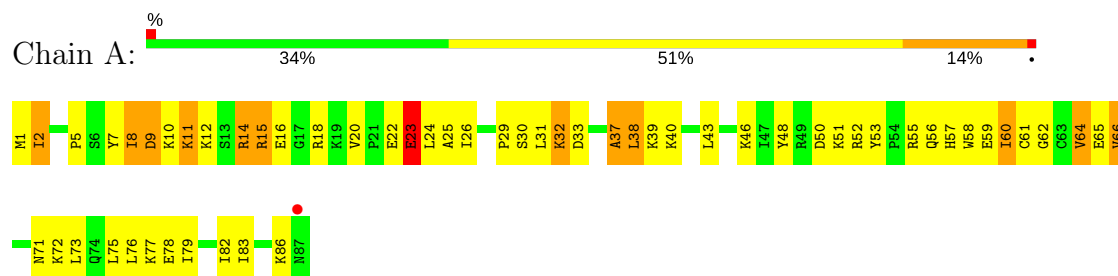
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	92	Total 92	O 92	0	0
4	N	119	Total 119	O 119	0	0

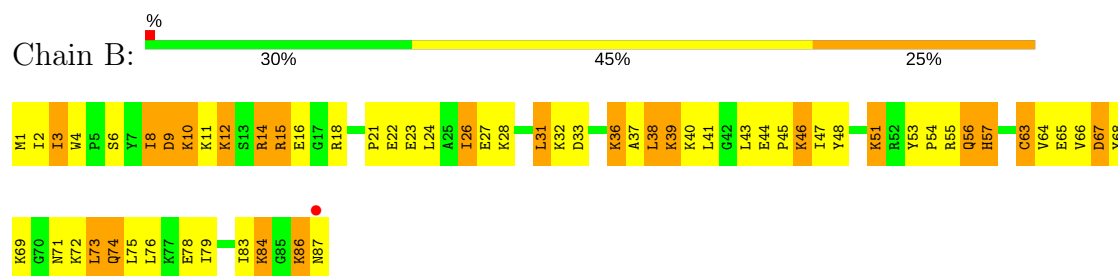
3 Residue-property plots

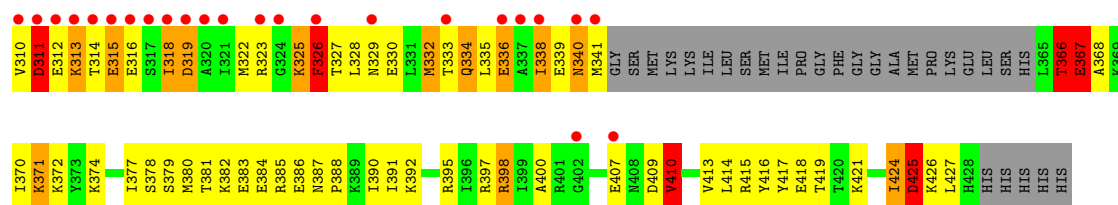
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN

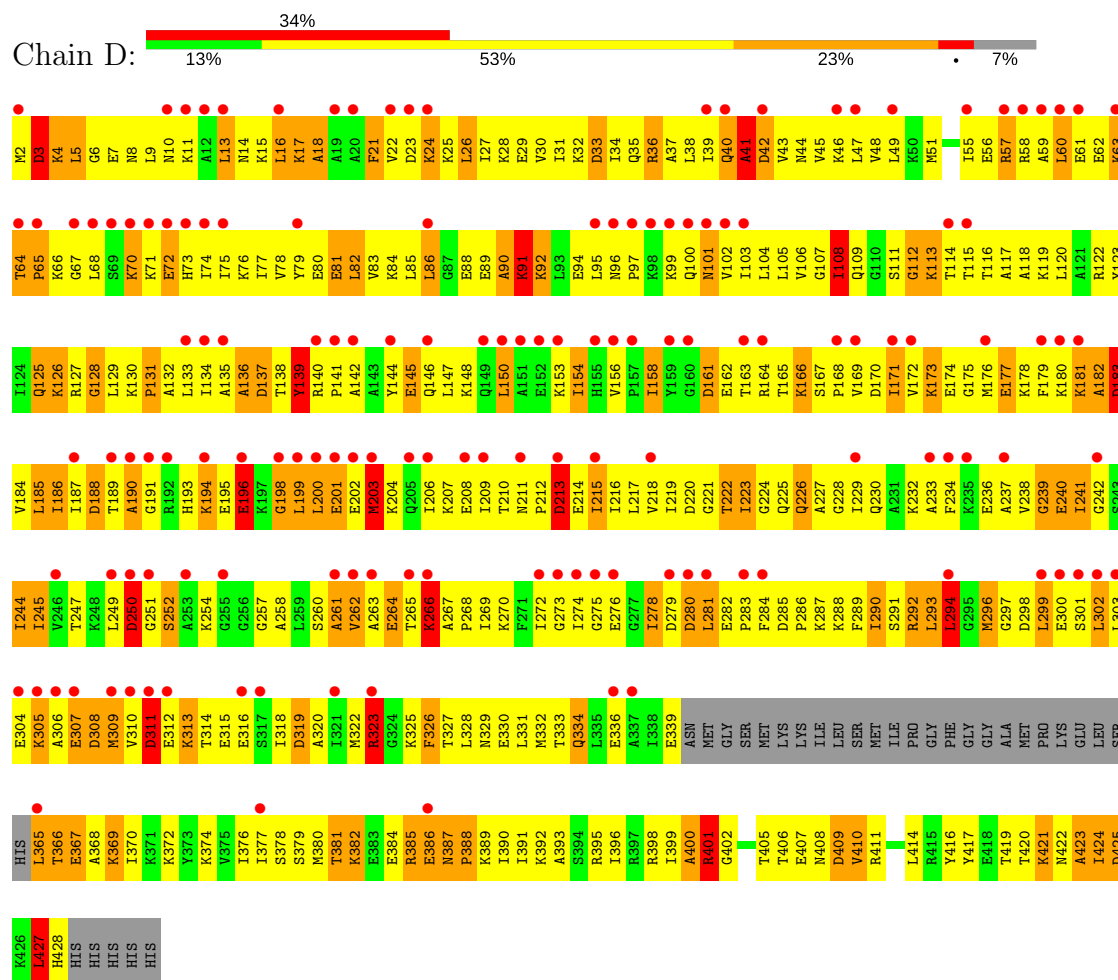


• Molecule 1: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN

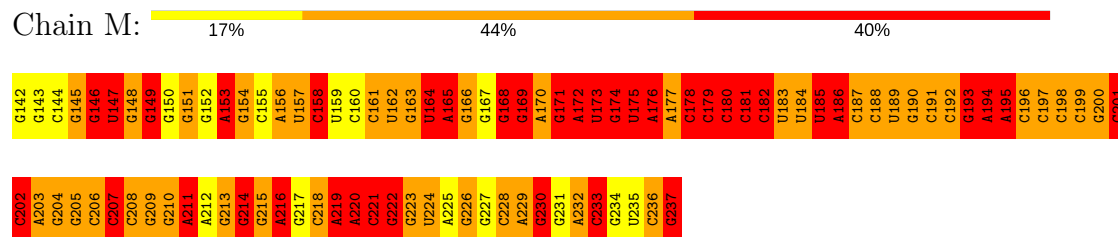




● Molecule 2: SIGNAL RECOGNITION 54 KDA PROTEIN



● Molecule 3: 7S RNA



● Molecule 3: 7S RNA



C202	C203	C204	G205	C206	C207	C208	C209	C210	A211	A212	C213	G214	G215	A216	C217	C218	A219	A220	C221	G222	G223	U224	A225	G226	C227	C228	A229	G230	C231	A232	C233	G234	U235	C236	C237																								
G142	G143	G144	G145	G146	U147	G148	G149	G150	G151	G152	A153	G154	C155	A156	U157	C158	U159	C160	C161	U162	G163	U164	A165	G166	G167	G168	G169	U170	C171	A172	U173	G174	U175	A176	A177	C178	C179	C180	C181	C182	U183	U184	U185	A186	C187	C188	U189	G190	C191	C192	G193	A194	A195	C196	C197	C198	C199	G200	C201

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.29Å 129.40Å 163.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 32.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 93.6 (32.35-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.244 , 0.294 0.263 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12336	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.55% 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, 0.333 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	1.19	1/740 (0.1%)	1.26	4/984 (0.4%)
1	B	1.15	1/740 (0.1%)	1.17	6/984 (0.6%)
2	C	0.83	1/3176 (0.0%)	1.05	16/4248 (0.4%)
2	D	0.63	0/3160	0.99	16/4227 (0.4%)
3	M	2.58	140/2309 (6.1%)	3.88	600/3603 (16.7%)
3	N	2.26	91/2309 (3.9%)	3.38	476/3603 (13.2%)
All	All	1.62	234/12434 (1.9%)	2.46	1118/17649 (6.3%)

The worst 5 of 234 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	218	C	N1-C6	-14.80	1.28	1.37
3	M	217	G	C8-N7	12.07	1.38	1.30
3	M	217	G	N7-C5	11.67	1.46	1.39
3	M	168	G	N3-C4	-11.48	1.27	1.35
3	N	172	A	N9-C4	11.11	1.44	1.37

The worst 5 of 1118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	209	G	C5-C6-O6	-24.70	113.78	128.60
3	M	194	A	O4'-C1'-N9	-20.43	91.86	108.20
3	M	217	G	C5-C6-O6	-20.20	116.48	128.60
3	N	217	G	C5-C6-O6	-19.78	116.73	128.60
3	M	142	G	O4'-C1'-N9	-18.30	93.56	108.20

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	727	0	786	80	0
1	B	727	0	786	90	0
2	C	3149	0	3364	579	0
2	D	3133	0	3349	620	0
3	M	2063	0	1043	162	0
3	N	2063	0	1041	136	0
4	A	23	0	0	2	0
4	B	26	0	0	2	0
4	C	107	0	0	17	0
4	D	107	0	0	21	0
4	M	92	0	0	11	0
4	N	119	0	0	4	0
All	All	12336	0	10369	1633	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 75.

The worst 5 of 1633 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:D:18:ALA:CB	2:D:71:LYS:HD2	1.54	1.34
2:C:325:LYS:HA	2:C:325:LYS:NZ	1.51	1.21
2:D:18:ALA:HB1	2:D:71:LYS:CD	1.71	1.19
2:D:290:ILE:HG23	2:D:294:LEU:HD21	1.22	1.18
2:C:64:THR:HG22	2:C:66:LYS:HB2	1.25	1.15

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	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	4	5
1	B	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	2	1
2	C	400/432 (93%)	258 (64%)	97 (24%)	45 (11%)	0	0
2	D	398/432 (92%)	227 (57%)	116 (29%)	55 (14%)	0	0
All	All	968/1038 (93%)	621 (64%)	239 (25%)	108 (11%)	0	0

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	18	ALA
2	C	19	ALA
2	C	24	LYS
2	C	64	THR
2	C	68	LEU

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	80/80 (100%)	69 (86%)	11 (14%)	4	8
1	B	80/80 (100%)	63 (79%)	17 (21%)	1	2
2	C	340/364 (93%)	264 (78%)	76 (22%)	1	1
2	D	338/364 (93%)	253 (75%)	85 (25%)	0	1
All	All	838/888 (94%)	649 (77%)	189 (23%)	1	1

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	303	LEU
2	D	4	LYS
2	D	327	THR

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Mol	Chain	Res	Type
2	C	313	LYS
2	C	334	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	334	GLN
2	C	340	ASN
2	D	101	ASN
2	C	329	ASN
2	D	226	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	95/96 (98%)	52 (54%)	0
3	N	95/96 (98%)	41 (43%)	0
All	All	190/192 (98%)	93 (48%)	0

5 of 93 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	M	145	G
3	M	146	G
3	M	147	U
3	M	149	G
3	M	153	A

There are no RNA pucker outliers to report.

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 [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	A	87/87 (100%)	0.28	1 (1%) 80 81	27, 42, 50, 53	0
1	B	87/87 (100%)	0.22	1 (1%) 80 81	27, 42, 53, 62	0
2	C	404/432 (93%)	1.00	75 (18%) 1 1	29, 57, 77, 88	0
2	D	402/432 (93%)	1.90	147 (36%) 0 0	31, 67, 80, 89	0
3	M	96/96 (100%)	-0.57	0 100 100	18, 37, 50, 61	0
3	N	96/96 (100%)	-0.53	0 100 100	20, 37, 52, 70	0
All	All	1172/1230 (95%)	0.94	224 (19%) 1 1	18, 56, 77, 89	0

The worst 5 of 224 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	280	ASP	13.0
2	D	251	GLY	12.9
2	D	301	SER	12.0
2	D	141	PRO	11.7
2	C	314	THR	10.8

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 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.