



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:05 am BST

PDB ID : 3KTW  
Title : Crystal structure of the SRP19/S-domain SRP RNA complex of *Sulfolobus solfataricus*  
Authors : Wild, K.; Bange, G.; Bozkurt, G.; Sinning, I.  
Deposited on : 2009-11-26  
Resolution : 3.20 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](mailto: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 ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

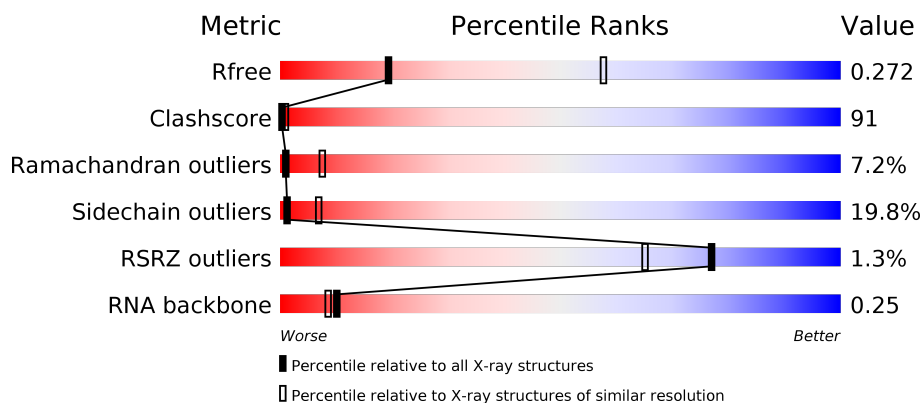
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	C	96	
1	D	96	
2	A	109	
2	B	109	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	C	10	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules 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 RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	96	Total	C	N	O	P	0	0	0
			2063	919	382	667	95			
1	D	95	Total	C	N	O	P	0	0	0
			2043	910	379	660	94			

- Molecule 2 is a protein called Signal recognition particle 19 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	92	Total	C	N	O	S	0	0	0
			766	496	139	130	1			
2	B	93	Total	C	N	O	S	0	0	0
			771	499	140	131	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	INSERTION	UNP Q980W2
A	-5	GLY	-	INSERTION	UNP Q980W2
A	-4	HIS	-	INSERTION	UNP Q980W2
A	-3	HIS	-	INSERTION	UNP Q980W2
A	-2	HIS	-	INSERTION	UNP Q980W2
A	-1	HIS	-	INSERTION	UNP Q980W2
A	0	HIS	-	INSERTION	UNP Q980W2
A	1	HIS	-	INSERTION	UNP Q980W2
B	-6	MET	-	INSERTION	UNP Q980W2
B	-5	GLY	-	INSERTION	UNP Q980W2
B	-4	HIS	-	INSERTION	UNP Q980W2
B	-3	HIS	-	INSERTION	UNP Q980W2
B	-2	HIS	-	INSERTION	UNP Q980W2
B	-1	HIS	-	INSERTION	UNP Q980W2
B	0	HIS	-	INSERTION	UNP Q980W2
B	1	HIS	-	INSERTION	UNP Q980W2

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		

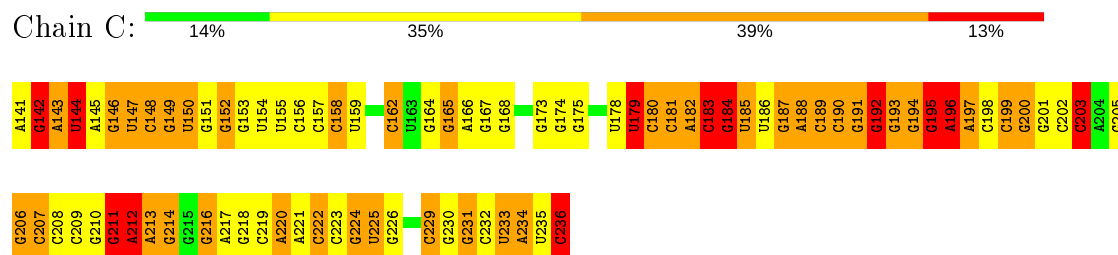
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	3	Total	Mg	0	0
			3	3		

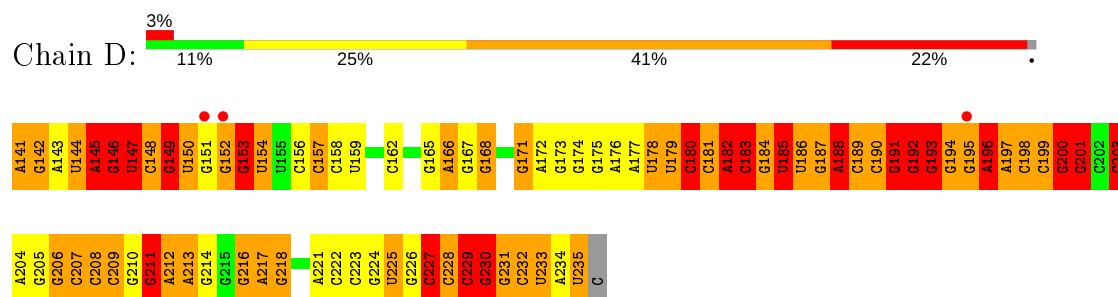
### 3 Residue-property plots [i](#)

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



- Molecule 1: SRP RNA



E57	M58	K59	K60	Y61	P62	R63	D64	R65	K66	I67	M68	F69	L70	I71	A72	V73	K74	K75	V76	K77	S78	K79		T82	L83	K84	I85	I86	H87	N88		T93	R94	GLN	THR	ASN	PRO	ASN	LYS	SER	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.31Å 79.34Å 114.07Å 90.00° 101.99° 90.00°	Depositor
Resolution (Å)	64.68 – 3.20 52.38 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (64.68-3.20) 98.9 (52.38-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.240 , 0.285 0.231 , 0.272	Depositor DCC
$R_{free}$ test set	1054 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.9	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG

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	1.48	32/2309 (1.4%)	1.80	66/3603 (1.8%)
1	D	1.98	56/2287 (2.4%)	1.89	98/3569 (2.7%)
2	A	0.54	1/780 (0.1%)	0.65	0/1047
2	B	0.66	2/785 (0.3%)	0.72	0/1054
All	All	1.54	91/6161 (1.5%)	1.66	164/9273 (1.8%)

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	C	0	2
1	D	0	5
All	All	0	7

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	G	C2-N2	36.95	1.71	1.34
1	D	187	G	C6-N1	22.44	1.55	1.39
1	D	149	G	C8-N7	22.36	1.44	1.30
1	C	183	C	N3-C4	-19.30	1.20	1.33
1	C	143	A	N7-C5	18.63	1.50	1.39

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	C	C5-C6-N1	-20.62	110.69	121.00
1	D	188	A	N1-C2-N3	-14.71	121.95	129.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	G	C5-C6-O6	14.12	137.07	128.60
1	C	182	A	C8-N9-C4	-13.86	100.26	105.80
1	D	149	G	C8-N9-C4	-13.41	101.04	106.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	183	C	Sidechain
1	C	184	G	Sidechain
1	D	146	G	Sidechain
1	D	188	A	Sidechain
1	D	191	G	Sidechain

## 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	C	2063	0	1036	314	4
1	D	2043	0	1024	283	4
2	A	766	0	828	138	0
2	B	771	0	830	125	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
All	All	5653	0	3718	833	4

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 91.

The worst 5 of 833 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:C:196:A:H5''	1:C:196:A:C8	1.21	1.60
1:D:146:G:N2	1:D:146:G:C2	1.71	1.54
1:C:233:U:O2	1:C:234:A:C8	1.72	1.40
2:A:51:LEU:HD22	2:A:73:VAL:CG1	1.53	1.38
1:C:186:U:O2	1:C:188:A:H5''	1.25	1.34

All (4) 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:C:141:A:N3	1:D:141:A:N6[1_656]	1.70	0.50
1:C:141:A:N3	1:D:141:A:N1[1_656]	1.87	0.33
1:C:141:A:N3	1:D:141:A:C6[1_656]	1.88	0.32
1:C:141:A:C4	1:D:141:A:N6[1_656]	1.98	0.22

## 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	
2	A	90/109 (83%)	65 (72%)	18 (20%)	7 (8%)	1	6
2	B	91/109 (84%)	69 (76%)	16 (18%)	6 (7%)	1	9
All	All	181/218 (83%)	134 (74%)	34 (19%)	13 (7%)	1	7

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	6	LEU
2	A	43	VAL
2	B	31	ALA
2	B	65	ARG
2	A	35	TYR

### 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	
2	A	86/102 (84%)	67 (78%)	19 (22%)	1	4
2	B	86/102 (84%)	71 (83%)	15 (17%)	2	10
All	All	172/204 (84%)	138 (80%)	34 (20%)	1	7

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	70	LEU
2	B	13	VAL
2	B	68	ASN
2	A	76	VAL
2	A	13	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	ASN
2	B	88	ASN
2	B	58	ASN
2	A	80	ASN
2	B	80	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	95/96 (98%)	33 (34%)	4 (4%)
1	D	95/96 (98%)	48 (50%)	8 (8%)
All	All	190/192 (98%)	81 (42%)	12 (6%)

5 of 81 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	142	G
1	C	144	U
1	C	146	G
1	C	147	U
1	C	148	C

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	145	A
1	D	178	U
1	D	196	A
1	D	141	A
1	D	195	G

## 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](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	96/96 (100%)	-0.22	0 <span>100</span> <span>100</span>	40, 82, 142, 151	0
1	D	95/96 (98%)	0.07	3 (3%) <span>47</span> <span>31</span>	37, 95, 175, 183	0
2	A	92/109 (84%)	-0.22	1 (1%) <span>80</span> <span>69</span>	48, 66, 87, 89	0
2	B	93/109 (85%)	-0.07	1 (1%) <span>80</span> <span>69</span>	39, 54, 69, 70	0
All	All	376/410 (91%)	-0.11	5 (1%) <span>77</span> <span>65</span>	37, 65, 161, 183	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	SER	5.1
2	A	2	SER	4.4
1	D	152	G	3.2
1	D	151	G	2.3
1	D	195	G	2.2

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	C	10	1/1	0.42	0.53	131,131,131,131	0
4	MG	D	9	1/1	0.71	0.32	69,69,69,69	0
3	K	D	4	1/1	0.79	0.24	103,103,103,103	0
4	MG	A	103	1/1	0.89	0.17	53,53,53,53	0
4	MG	C	8	1/1	0.91	0.35	79,79,79,79	0
4	MG	B	103	1/1	0.91	0.45	57,57,57,57	0
3	K	D	1	1/1	0.94	0.38	82,82,82,82	0
3	K	C	3	1/1	0.96	0.47	84,84,84,84	0
3	K	C	2	1/1	0.98	0.43	73,73,73,73	0
4	MG	C	6	1/1	0.98	0.27	52,52,52,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.