



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:56 PM GMT

PDB ID : 1Z63  
Title : Sulfolobus solfataricus SWI2/SNF2 ATPase core in complex with dsDNA  
Authors : Duerr, H.; Koerner, C.; Mueller, M.; Hickmann, V.; Hopfner, K.P.  
Deposited on : 2005-03-21  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

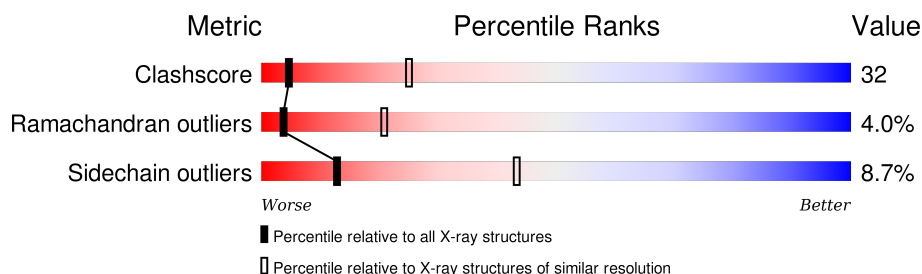
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	25	
1	E	25	
2	D	25	
2	F	25	
3	A	500	
3	B	500	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9154 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 DNA chain called 5'-D(\*AP\*AP\*AP\*AP\*AP\*A\*AP\*TP\*TP\*GP\*CP\*CP\*GP\*AP\*AP\*GP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	19	Total	C	N	O	P	16	0	0
			392	187	83	104	18			
1	E	19	Total	C	N	O	P	0	0	0
			392	187	83	104	18			

- Molecule 2 is a DNA chain called 5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*CP\*GP\*TP\*CP\*TP\*TP\*CP\*GP\*GP\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	P	0	0	0
			401	196	59	127	19			
2	F	20	Total	C	N	O	P	0	0	0
			401	196	59	127	19			

- Molecule 3 is a protein called Helicase of the snf2/rad54 family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	468	Total	C	N	O	S	Se	0	0	0
			3784	2440	636	695	3	10			
3	B	468	Total	C	N	O	S	Se	0	0	0
			3784	2440	636	695	3	10			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	MET	-	EXPRESSION TAG	UNP Q97XQ5
A	408	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	409	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	410	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	411	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	412	HIS	-	EXPRESSION TAG	UNP Q97XQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	413	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	414	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	415	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	416	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	417	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	418	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	419	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	420	LEU	-	EXPRESSION TAG	UNP Q97XQ5
A	421	VAL	-	EXPRESSION TAG	UNP Q97XQ5
A	422	PRO	-	EXPRESSION TAG	UNP Q97XQ5
A	423	ARG	-	EXPRESSION TAG	UNP Q97XQ5
A	424	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	425	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	426	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	427	MET	-	EXPRESSION TAG	UNP Q97XQ5
A	428	ALA	-	EXPRESSION TAG	UNP Q97XQ5
A	429	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	497	VAL	-	EXPRESSION TAG	UNP Q97XQ5
A	904	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	905	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	906	TYR	-	EXPRESSION TAG	UNP Q97XQ5
B	407	MET	-	EXPRESSION TAG	UNP Q97XQ5
B	408	GLY	-	EXPRESSION TAG	UNP Q97XQ5
B	409	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	410	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	411	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	412	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	413	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	414	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	415	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	416	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	417	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	418	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	419	GLY	-	EXPRESSION TAG	UNP Q97XQ5
B	420	LEU	-	EXPRESSION TAG	UNP Q97XQ5
B	421	VAL	-	EXPRESSION TAG	UNP Q97XQ5
B	422	PRO	-	EXPRESSION TAG	UNP Q97XQ5
B	423	ARG	-	EXPRESSION TAG	UNP Q97XQ5
B	424	GLY	-	EXPRESSION TAG	UNP Q97XQ5
B	425	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	426	HIS	-	EXPRESSION TAG	UNP Q97XQ5
B	427	MET	-	EXPRESSION TAG	UNP Q97XQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	428	ALA	-	EXPRESSION TAG	UNP Q97XQ5
B	429	SER	-	EXPRESSION TAG	UNP Q97XQ5
B	497	VAL	-	EXPRESSION TAG	UNP Q97XQ5
B	904	GLY	-	EXPRESSION TAG	UNP Q97XQ5
B	905	GLY	-	EXPRESSION TAG	UNP Q97XQ5
B	906	TYR	-	EXPRESSION TAG	UNP Q97XQ5

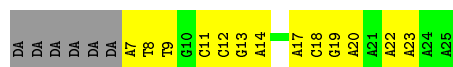
### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

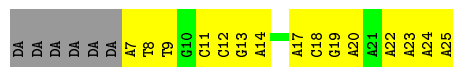
- Molecule 1: 5'-D(\*AP\*AP\*AP\*AP\*AP\*A\*AP\*TP\*TP\*GP\*CP\*CP\*GP\*AP\*AP\*GP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*AP\*A)-3'

Chain C: 



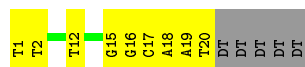
- Molecule 1: 5'-D(\*AP\*AP\*AP\*AP\*AP\*A\*AP\*TP\*TP\*GP\*CP\*CP\*GP\*AP\*AP\*GP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*AP\*A)-3'

Chain E: 



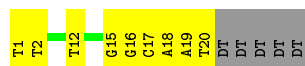
- Molecule 2: 5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*CP\*GP\*TP\*CP\*TP\*TP\*CP\*GP\*GP\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*TP\*T)-3'

Chain D: 



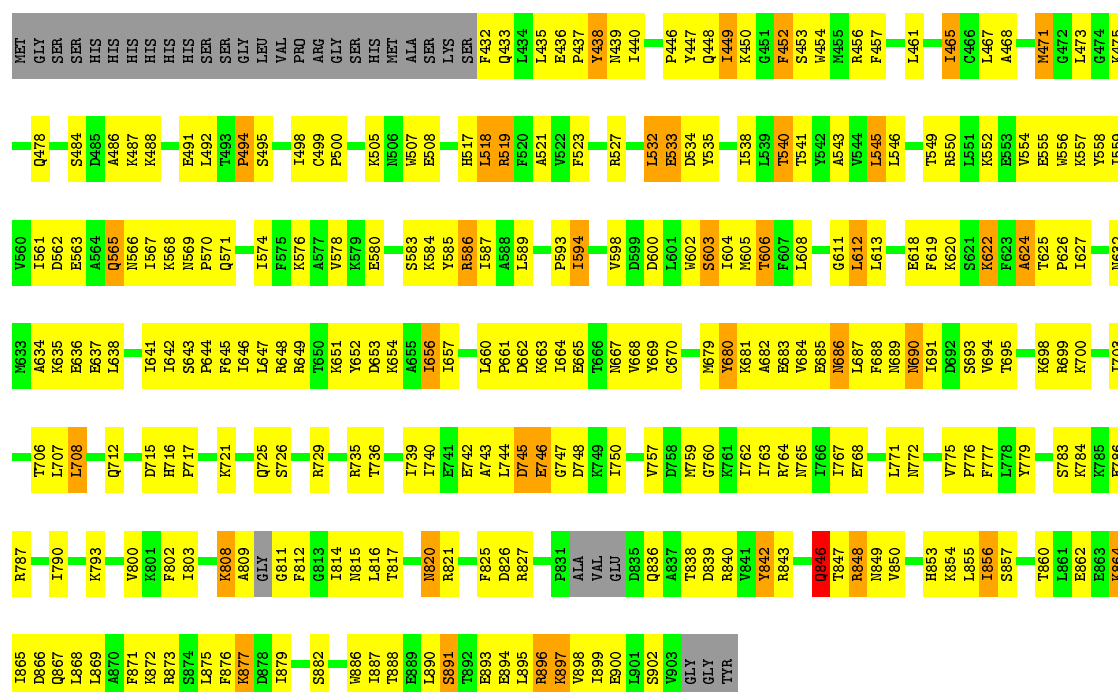
- Molecule 2: 5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*CP\*GP\*TP\*CP\*TP\*TP\*CP\*GP\*GP\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*TP\*T)-3'

Chain F: 

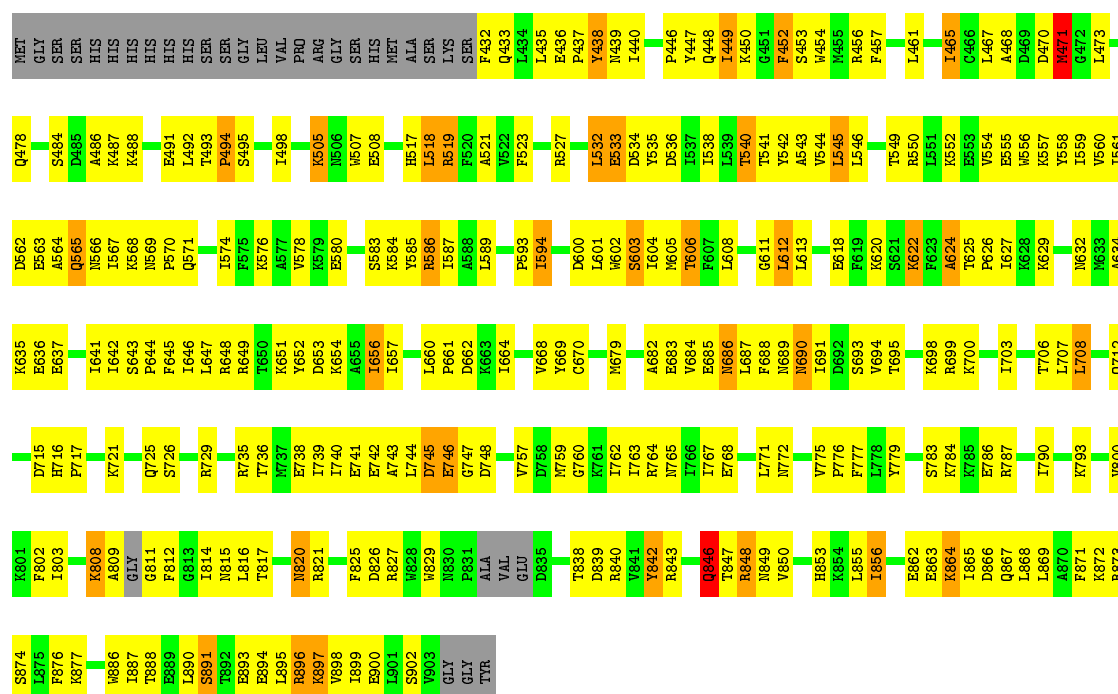


- Molecule 3: Helicase of the snf2/rad54 family

Chain A: 



### • Molecule 3: Helicase of the snf2/rad54 family



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.93 Å   83.74 Å   106.39 Å 90.00°   109.78°   90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP



## 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	0.62	0/443	0.79	0/682
1	E	0.63	0/443	0.81	0/682
2	D	0.55	0/445	0.83	0/685
2	F	0.60	0/445	0.83	0/685
3	A	0.61	0/3841	0.80	3/5156 (0.1%)
3	B	0.61	0/3841	0.80	2/5156 (0.0%)
All	All	0.61	0/9458	0.80	5/13046 (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
3	A	0	1
3	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	842	TYR	N-CA-C	-6.15	94.39	111.00
3	B	842	TYR	N-CA-C	-5.96	94.92	111.00
3	A	471	MSE	N-CA-C	-5.38	96.48	111.00
3	B	471	MSE	N-CA-C	-5.25	96.84	111.00
3	A	846	GLN	N-CA-C	5.06	124.67	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	669	TYR	Sidechain
3	B	669	TYR	Sidechain

## 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	392	0	213	19	0
1	E	392	0	213	20	0
2	D	401	0	233	11	0
2	F	401	0	233	12	0
3	A	3784	0	3912	260	0
3	B	3784	0	3912	261	0
All	All	9154	0	8716	571	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 32.

The worst 5 of 571 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:F:16:DG:H2''	2:F:17:DC:H5'	1.19	1.18
2:D:16:DG:H2''	2:D:17:DC:H5'	1.19	1.07
3:A:602:TRP:O	3:A:606:THR:HG22	1.64	0.97
3:B:602:TRP:O	3:B:606:THR:HG22	1.65	0.95
3:A:465:ILE:HD11	3:A:587:ILE:HG12	1.47	0.93

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	
3	A	462/500 (92%)	378 (82%)	65 (14%)	19 (4%)	3	20
3	B	462/500 (92%)	379 (82%)	65 (14%)	18 (4%)	4	21
All	All	924/1000 (92%)	757 (82%)	130 (14%)	37 (4%)	4	21

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	438	TYR
3	A	533	GLU
3	A	612	LEU
3	A	624	ALA
3	A	846	GLN

### 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	
3	A	421/436 (97%)	384 (91%)	37 (9%)	12	42
3	B	421/436 (97%)	385 (91%)	36 (9%)	13	44
All	All	842/872 (97%)	769 (91%)	73 (9%)	13	43

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	864	LYS
3	B	465	ILE
3	B	848	ARG
3	B	433	GLN
3	B	494	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	836	GLN
3	B	433	GLN
3	B	836	GLN
3	A	867	GLN
3	B	459	ASN

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.