W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:11 PM GMT

PDB ID	:	1SHS
Title	:	SMALL HEAT SHOCK PROTEIN FROM METHANOCOCCUS JAN-NASCHII
Authors	:	Kim, K.K.; Kim, R.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	1998-07-30
Resolution	:	2.90 Å(reported)

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 (i)

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.
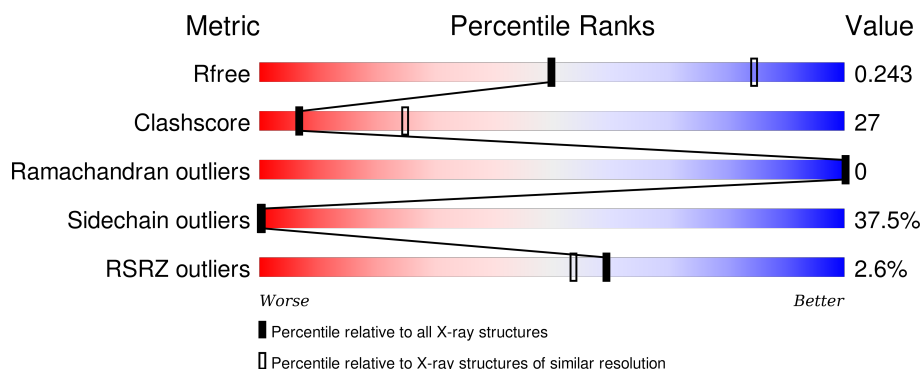
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 <=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	147	2% 29% 33% 17% 22%
1	B	147	% 33% 30% 15% 22%
1	C	147	3% 33% 29% 16% 22%
1	D	147	5% 34% 29% 15% 22%
1	E	147	2% 37% 28% 14% 22%

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Mol	Chain	Length	Quality of chain
1	F	147	% 38% 27% 13% 22%
1	G	147	% 36% 27% 15% 22%
1	H	147	2% 37% 28% 14% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7144 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 SMALL HEAT SHOCK PROTEIN.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			
1	B	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			
1	C	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			
1	D	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			
1	E	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			
1	F	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			
1	G	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			
1	H	115	Total	C	N	O	S	0	0	0
			893	570	147	174	2			

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 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: SMALL HEAT SHOCK PROTEIN
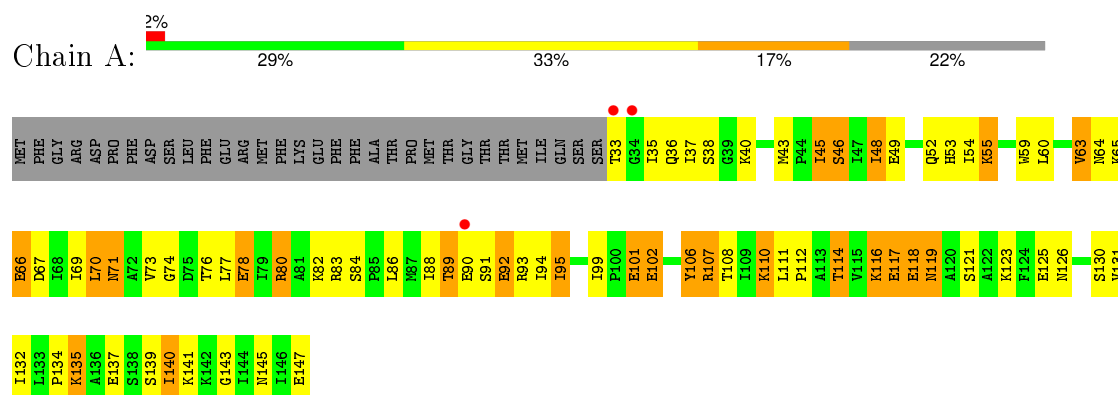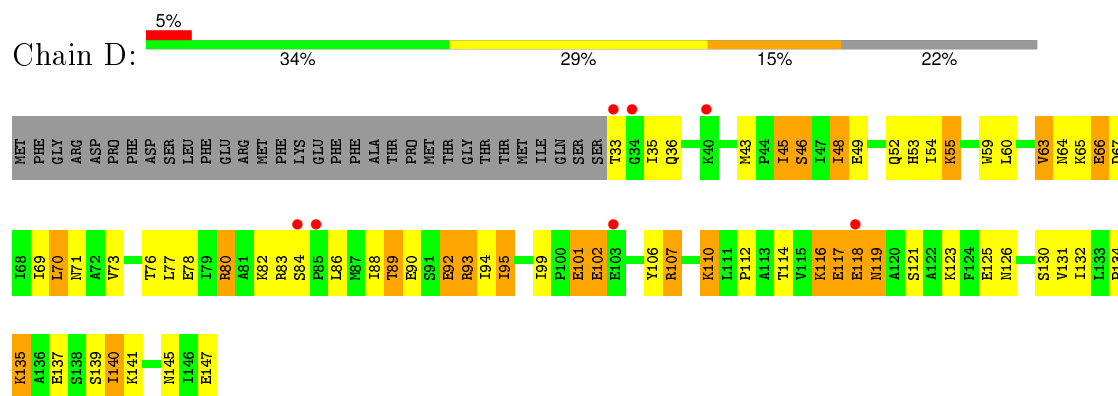
Chain A:

• Molecule 1: SMALL HEAT SHOCK PROTEIN

Chain B:

• Molecule 1: SMALL HEAT SHOCK PROTEIN

Chain C:

• Molecule 1: SMALL HEAT SHOCK PROTEIN

Chain D:

• Molecule 1: SMALL HEAT SHOCK PROTEIN

Chain E:

• Molecule 1: SMALL HEAT SHOCK PROTEIN

Chain F:

• Molecule 1: SMALL HEAT SHOCK PROTEIN

Chain G:
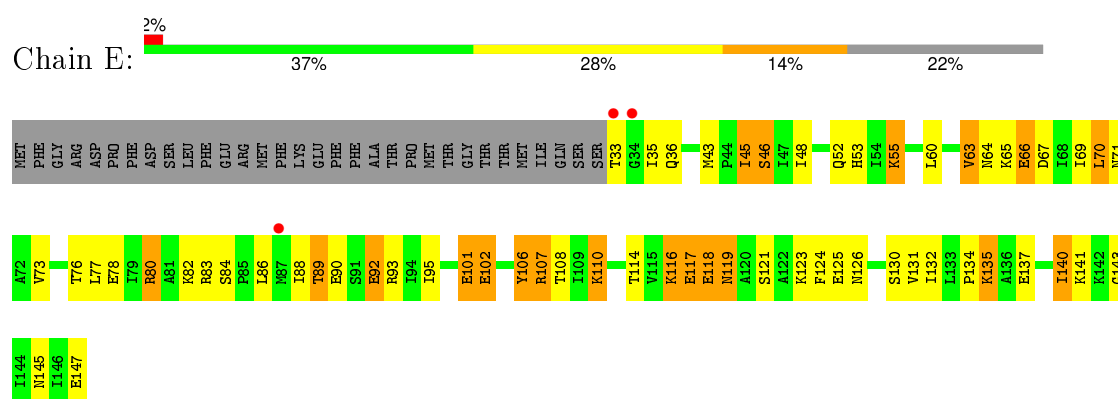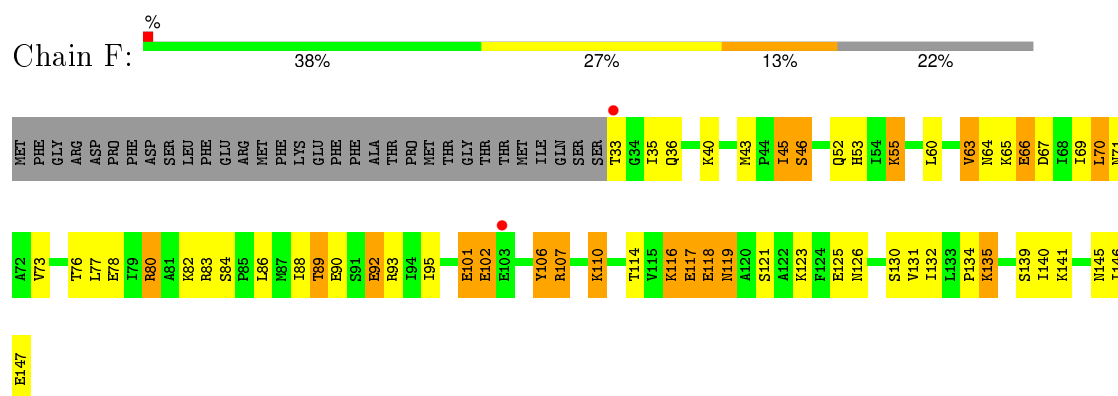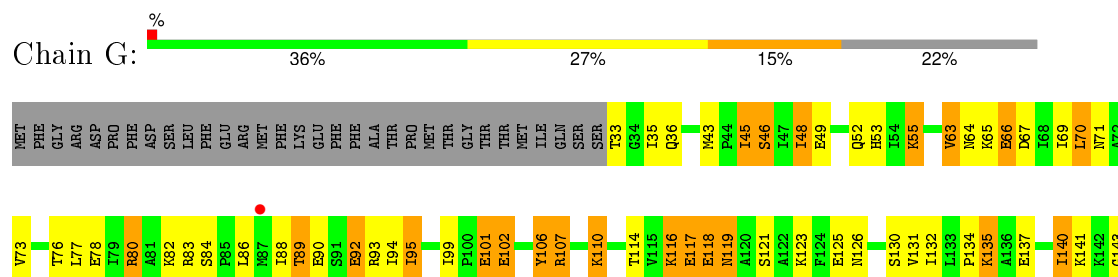
I144 N145 I146 E147

• Molecule 1: SMALL HEAT SHOCK PROTEIN

Chain H:

2%

37%   28%   14%   22%

MET PHE GLY ARG ASP PRO PHE ASP SER LEU PHE GLU ARG MET PHE LYS GLU PHE ALA THR PRO MET THR GLY THR THR MET ILE GLN SER SER T33 G34 I35 Q36 M43 P44 I45 S46 I47 I48 E49 H53 I54 K55 L60 V63 N64 K65 E66 D67 I68 I69 L70 N71

A72 V73 T76 L77 E78 I79 R80 A81 K82 R83 S84 P85 L86 M87 I88 T89 E90 S91 E92 R93 I94 I95 I99 P100 E101 E102 E103 Y106 R107 T108 I109 K110 L111 P112 A113 T114 V115 K116 E117 E118 N119 A120 S121 A122 K123 S130 V131 I132 L133 P134 K135 S139 I140 N145

I146 E147

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	171.44Å 171.44Å 101.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.90 28.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.6 (15.00-2.90) 96.7 (28.57-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.90Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.216 , 0.251 0.222 , 0.243	Depositor DCC
R_{free} test set	2350 reflections (9.88%)	DCC
Wilson B-factor (Å^2)	83.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 62.6	EDS
Estimated twinning fraction	0.000 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.000 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.000 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.000 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.007 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| >$ = 0.51, $< L^2 >$ = 0.35	Xtriage
Outliers	0 of 24688 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7144	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.59	0/905	0.73	0/1221
1	B	0.55	0/905	0.74	0/1221
1	C	0.63	0/905	0.73	0/1221
1	D	0.58	0/905	0.73	0/1221
1	E	0.58	0/905	0.72	0/1221
1	F	0.55	0/905	0.73	0/1221
1	G	0.62	0/905	0.73	0/1221
1	H	0.58	0/905	0.73	0/1221
All	All	0.59	0/7240	0.73	0/9768

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	893	0	932	66	0
1	B	893	0	932	67	0
1	C	893	0	932	60	0
1	D	893	0	932	56	0
1	E	893	0	932	46	0
1	F	893	0	932	47	0
1	G	893	0	932	53	0
1	H	893	0	932	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7144	0	7456	393	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 27.

The worst 5 of 393 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:107:ARG:HH11	1:C:107:ARG:HG2	1.42	0.85
1:F:63:VAL:HG23	1:F:83:ARG:HB3	1.60	0.84
1:E:107:ARG:HH11	1:E:107:ARG:HG2	1.44	0.82
1:B:141:LYS:HA	1:F:73:VAL:HB	1.61	0.82
1:B:93:ARG:CZ	1:H:80:ARG:HH21	1.92	0.81

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	A	113/147 (77%)	107 (95%)	6 (5%)	0	100	100
1	B	113/147 (77%)	108 (96%)	5 (4%)	0	100	100
1	C	113/147 (77%)	107 (95%)	6 (5%)	0	100	100
1	D	113/147 (77%)	108 (96%)	5 (4%)	0	100	100
1	E	113/147 (77%)	106 (94%)	7 (6%)	0	100	100
1	F	113/147 (77%)	107 (95%)	6 (5%)	0	100	100
1	G	113/147 (77%)	106 (94%)	7 (6%)	0	100	100
1	H	113/147 (77%)	107 (95%)	6 (5%)	0	100	100
All	All	904/1176 (77%)	856 (95%)	48 (5%)	0	100	100

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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	100/129 (78%)	62 (62%)	38 (38%)	0	0
1	B	100/129 (78%)	63 (63%)	37 (37%)	0	0
1	C	100/129 (78%)	62 (62%)	38 (38%)	0	0
1	D	100/129 (78%)	62 (62%)	38 (38%)	0	0
1	E	100/129 (78%)	63 (63%)	37 (37%)	0	0
1	F	100/129 (78%)	63 (63%)	37 (37%)	0	0
1	G	100/129 (78%)	63 (63%)	37 (37%)	0	0
1	H	100/129 (78%)	62 (62%)	38 (38%)	0	0
All	All	800/1032 (78%)	500 (62%)	300 (38%)	0	0

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	106	TYR
1	E	90	GLU
1	H	89	THR
1	D	116	LYS
1	E	46	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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(Å²)	Q<0.9
1	A	115/147 (78%)	-0.05	3 (2%)	59 54	32, 57, 86, 100	0
1	B	115/147 (78%)	-0.19	1 (0%)	85 84	38, 56, 86, 95	0
1	C	115/147 (78%)	-0.01	4 (3%)	48 40	30, 52, 86, 98	0
1	D	115/147 (78%)	0.08	7 (6%)	25 18	35, 56, 87, 98	0
1	E	115/147 (78%)	-0.19	3 (2%)	59 54	36, 56, 88, 98	0
1	F	115/147 (78%)	-0.15	2 (1%)	73 70	40, 58, 87, 95	0
1	G	115/147 (78%)	-0.21	1 (0%)	85 84	28, 52, 86, 96	0
1	H	115/147 (78%)	-0.14	3 (2%)	59 54	35, 55, 86, 97	0
All	All	920/1176 (78%)	-0.11	24 (2%)	59 54	28, 56, 88, 100	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	GLU	5.0
1	A	33	THR	4.8
1	H	33	THR	4.4
1	H	34	GLY	3.8
1	D	85	PRO	3.7

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.