



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:29 PM GMT

PDB ID : 3ZHA  
Title : Molecular basis for the action of the collagen-specific chaperone Hsp47 SER-PINH1 and its structure-specific client recognition.  
Authors : Widmer, C.; Gebauer, J.M.; Baumann, U.  
Deposited on : 2012-12-20  
Resolution : 2.55 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) : 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

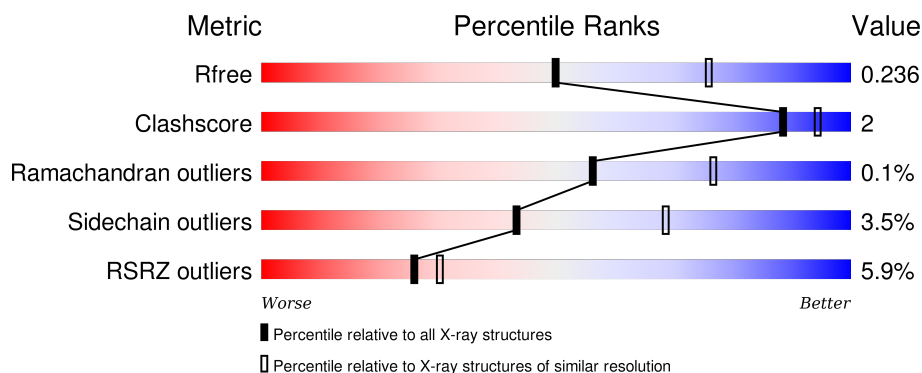
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div>7%</div> <div>89% 8% . .</div> </div>
1	B	392	<div> <div>5%</div> <div>85% 7% . 7%</div> </div>
1	C	392	<div> <div>10%</div> <div>89% 7% .</div> </div>
1	D	392	<div> <div>6%</div> <div>86% 7% . 6%</div> </div>
1	K	392	<div> <div>4%</div> <div>88% 7% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	392	
1	P	392	
1	Q	392	
2	E	19	
2	F	19	
2	G	19	
2	H	19	
2	I	19	
2	J	19	
2	M	19	
2	N	19	
2	O	19	
2	R	19	
2	S	19	
2	T	19	

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
3	SIN	A	1421	-	-	-	X
3	SIN	C	1418	-	-	-	X
3	SIN	K	1415	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24911 atoms, of which 8 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 HSP47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2981	1898	517	552	14			
1	B	364	Total	C	N	O	S	0	0	0
			2855	1820	496	526	13			
1	C	376	Total	C	N	O	S	0	0	0
			2961	1884	516	548	13			
1	D	368	Total	C	N	O	S	0	0	0
			2894	1840	506	535	13			
1	K	374	Total	C	N	O	S	0	0	0
			2955	1879	515	547	14			
1	L	369	Total	C	N	O	S	0	0	0
			2902	1847	505	537	13			
1	P	373	Total	C	N	O	S	0	0	0
			2938	1868	511	546	13			
1	Q	365	Total	C	N	O	S	0	0	0
			2872	1828	500	531	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	EXPRESSION TAG	UNP C7C419
A	419	LEU	-	EXPRESSION TAG	UNP C7C419
A	420	GLU	-	EXPRESSION TAG	UNP C7C419
A	421	HIS	-	EXPRESSION TAG	UNP C7C419
A	422	HIS	-	EXPRESSION TAG	UNP C7C419
A	423	HIS	-	EXPRESSION TAG	UNP C7C419
A	424	HIS	-	EXPRESSION TAG	UNP C7C419
A	425	HIS	-	EXPRESSION TAG	UNP C7C419
A	426	HIS	-	EXPRESSION TAG	UNP C7C419
B	35	MET	-	EXPRESSION TAG	UNP C7C419
B	419	LEU	-	EXPRESSION TAG	UNP C7C419
B	420	GLU	-	EXPRESSION TAG	UNP C7C419
B	421	HIS	-	EXPRESSION TAG	UNP C7C419

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	HIS	-	EXPRESSION TAG	UNP C7C419
B	423	HIS	-	EXPRESSION TAG	UNP C7C419
B	424	HIS	-	EXPRESSION TAG	UNP C7C419
B	425	HIS	-	EXPRESSION TAG	UNP C7C419
B	426	HIS	-	EXPRESSION TAG	UNP C7C419
C	35	MET	-	EXPRESSION TAG	UNP C7C419
C	419	LEU	-	EXPRESSION TAG	UNP C7C419
C	420	GLU	-	EXPRESSION TAG	UNP C7C419
C	421	HIS	-	EXPRESSION TAG	UNP C7C419
C	422	HIS	-	EXPRESSION TAG	UNP C7C419
C	423	HIS	-	EXPRESSION TAG	UNP C7C419
C	424	HIS	-	EXPRESSION TAG	UNP C7C419
C	425	HIS	-	EXPRESSION TAG	UNP C7C419
C	426	HIS	-	EXPRESSION TAG	UNP C7C419
D	35	MET	-	EXPRESSION TAG	UNP C7C419
D	419	LEU	-	EXPRESSION TAG	UNP C7C419
D	420	GLU	-	EXPRESSION TAG	UNP C7C419
D	421	HIS	-	EXPRESSION TAG	UNP C7C419
D	422	HIS	-	EXPRESSION TAG	UNP C7C419
D	423	HIS	-	EXPRESSION TAG	UNP C7C419
D	424	HIS	-	EXPRESSION TAG	UNP C7C419
D	425	HIS	-	EXPRESSION TAG	UNP C7C419
D	426	HIS	-	EXPRESSION TAG	UNP C7C419
K	35	MET	-	EXPRESSION TAG	UNP C7C419
K	419	LEU	-	EXPRESSION TAG	UNP C7C419
K	420	GLU	-	EXPRESSION TAG	UNP C7C419
K	421	HIS	-	EXPRESSION TAG	UNP C7C419
K	422	HIS	-	EXPRESSION TAG	UNP C7C419
K	423	HIS	-	EXPRESSION TAG	UNP C7C419
K	424	HIS	-	EXPRESSION TAG	UNP C7C419
K	425	HIS	-	EXPRESSION TAG	UNP C7C419
K	426	HIS	-	EXPRESSION TAG	UNP C7C419
L	35	MET	-	EXPRESSION TAG	UNP C7C419
L	419	LEU	-	EXPRESSION TAG	UNP C7C419
L	420	GLU	-	EXPRESSION TAG	UNP C7C419
L	421	HIS	-	EXPRESSION TAG	UNP C7C419
L	422	HIS	-	EXPRESSION TAG	UNP C7C419
L	423	HIS	-	EXPRESSION TAG	UNP C7C419
L	424	HIS	-	EXPRESSION TAG	UNP C7C419
L	425	HIS	-	EXPRESSION TAG	UNP C7C419
L	426	HIS	-	EXPRESSION TAG	UNP C7C419
P	35	MET	-	EXPRESSION TAG	UNP C7C419

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Chain	Residue	Modelled	Actual	Comment	Reference
P	419	LEU	-	EXPRESSION TAG	UNP C7C419
P	420	GLU	-	EXPRESSION TAG	UNP C7C419
P	421	HIS	-	EXPRESSION TAG	UNP C7C419
P	422	HIS	-	EXPRESSION TAG	UNP C7C419
P	423	HIS	-	EXPRESSION TAG	UNP C7C419
P	424	HIS	-	EXPRESSION TAG	UNP C7C419
P	425	HIS	-	EXPRESSION TAG	UNP C7C419
P	426	HIS	-	EXPRESSION TAG	UNP C7C419
Q	35	MET	-	EXPRESSION TAG	UNP C7C419
Q	419	LEU	-	EXPRESSION TAG	UNP C7C419
Q	420	GLU	-	EXPRESSION TAG	UNP C7C419
Q	421	HIS	-	EXPRESSION TAG	UNP C7C419
Q	422	HIS	-	EXPRESSION TAG	UNP C7C419
Q	423	HIS	-	EXPRESSION TAG	UNP C7C419
Q	424	HIS	-	EXPRESSION TAG	UNP C7C419
Q	425	HIS	-	EXPRESSION TAG	UNP C7C419
Q	426	HIS	-	EXPRESSION TAG	UNP C7C419

- Molecule 2 is a protein called COLLAGEN MODEL PEPTIDE 18-T8R11.

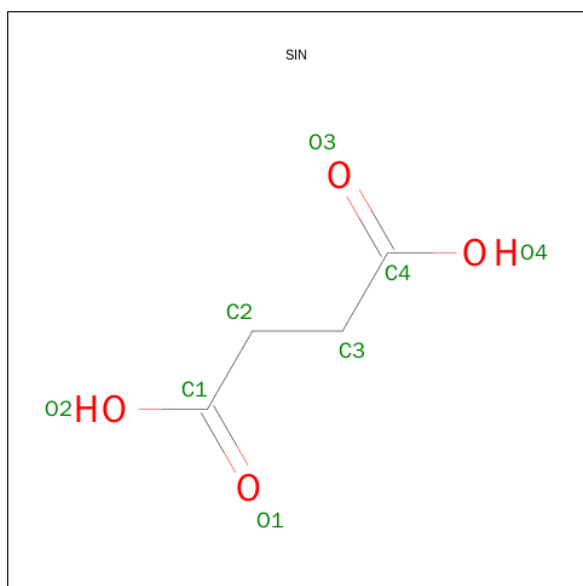
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	0	0	0
			111	72	20	19			
2	F	17	Total	C	N	O	0	0	0
			104	67	19	18			
2	G	16	Total	C	N	O	0	0	0
			97	62	18	17			
2	H	18	Total	C	N	O	0	0	0
			111	72	20	19			
2	I	17	Total	C	N	O	0	0	0
			104	67	19	18			
2	J	16	Total	C	N	O	0	0	0
			97	62	18	17			
2	M	18	Total	C	N	O	0	0	0
			111	72	20	19			
2	N	18	Total	C	N	O	0	0	0
			111	72	20	19			
2	O	18	Total	C	N	O	0	0	0
			111	72	20	19			
2	R	18	Total	C	N	O	0	0	0
			111	72	20	19			
2	S	18	Total	C	N	O	0	0	0
			111	72	20	19			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	T	17	Total	C	N	O	0	0	0
			104	67	19	18			

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			8	4	4			
3	C	1	Total	C	O		0	0
			8	4	4			
3	K	1	Total	C	O		0	0
			8	4	4			
3	P	1	Total	C	H	O	0	0
			12	4	4	4		
3	Q	1	Total	C	H	O	0	0
			12	4	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	21	Total	O	0	0
			21	21		
4	C	33	Total	O	0	0
			33	33		

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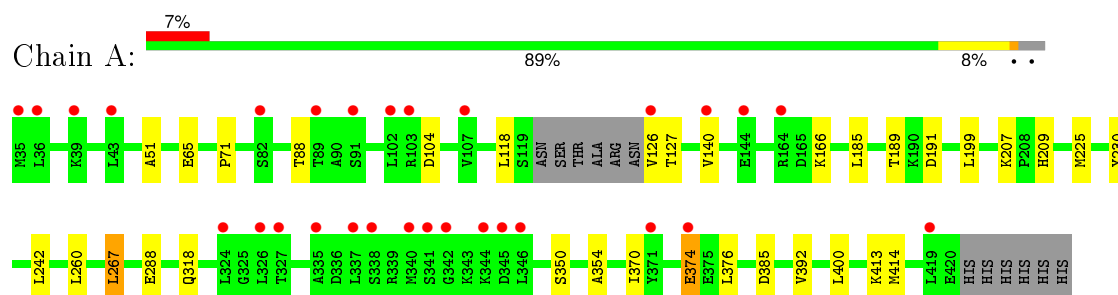
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	37	Total 37	O 37	0	0
4	E	2	Total 2	O 2	0	0
4	F	1	Total 1	O 1	0	0
4	I	2	Total 2	O 2	0	0
4	K	24	Total 24	O 24	0	0
4	L	27	Total 27	O 27	0	0
4	N	3	Total 3	O 3	0	0
4	P	18	Total 18	O 18	0	0
4	Q	27	Total 27	O 27	0	0
4	R	1	Total 1	O 1	0	0
4	S	2	Total 2	O 2	0	0
4	T	1	Total 1	O 1	0	0



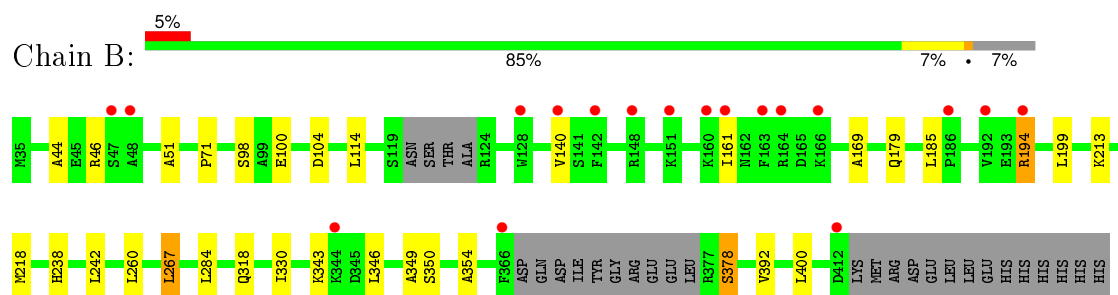
### 3 Residue-property plots

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

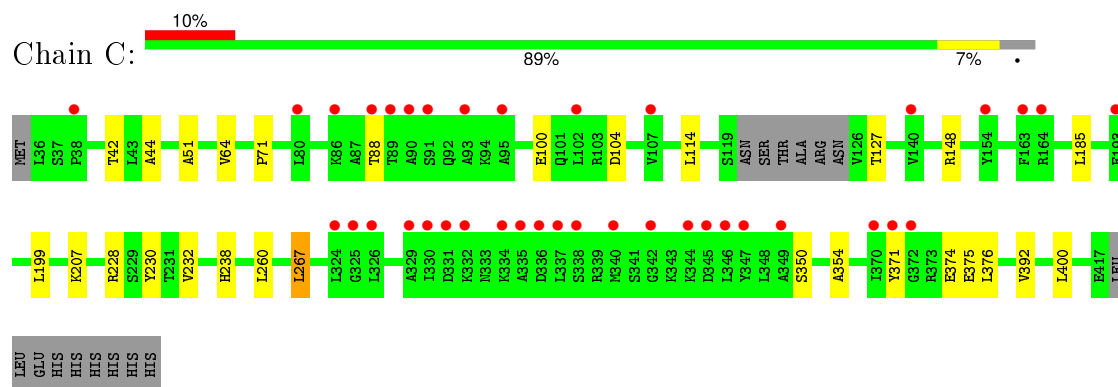
#### • Molecule 1: HSP47



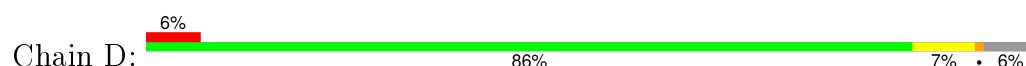
#### • Molecule 1: HSP47

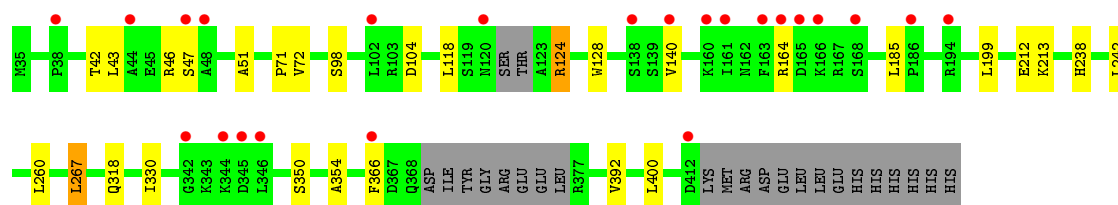


#### • Molecule 1: HSP47

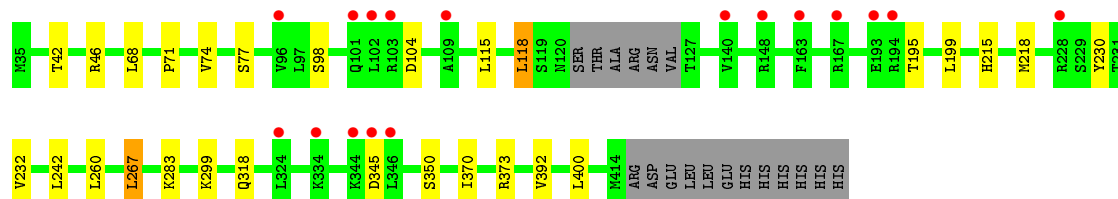
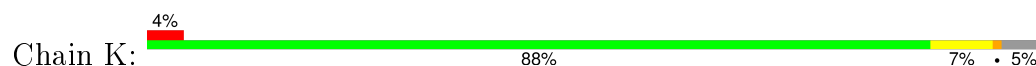


#### • Molecule 1: HSP47

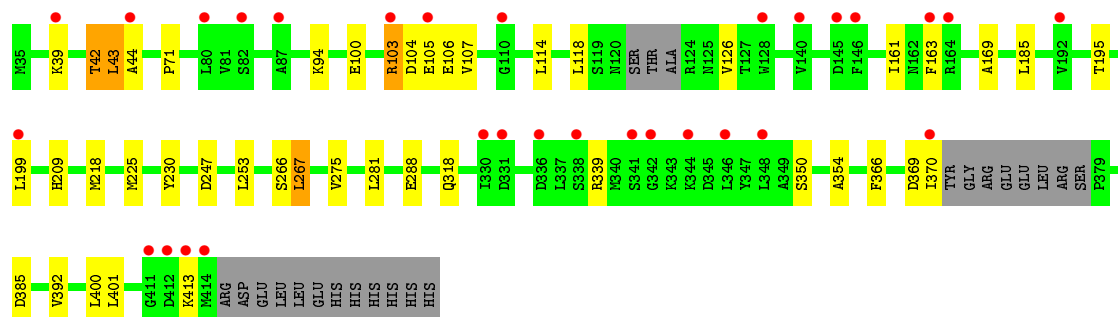
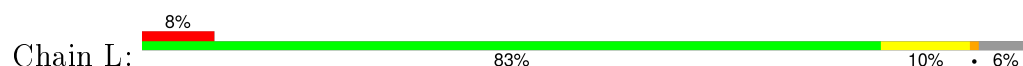




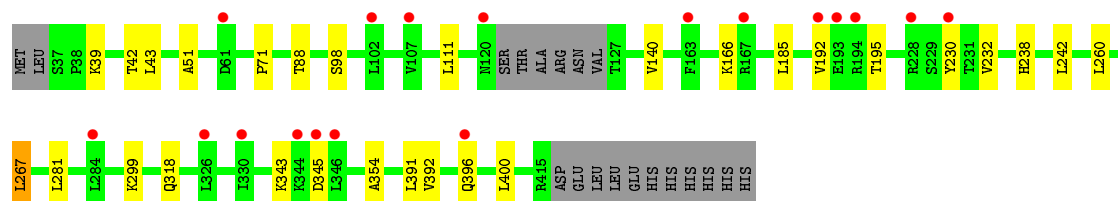
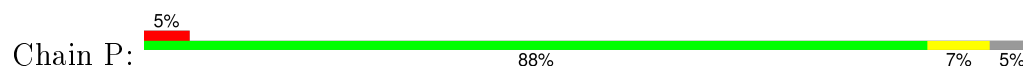
• Molecule 1: HSP47



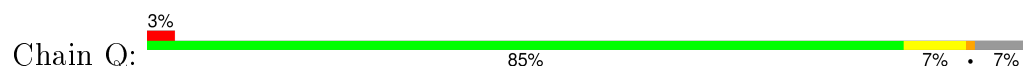
• Molecule 1: HSP47

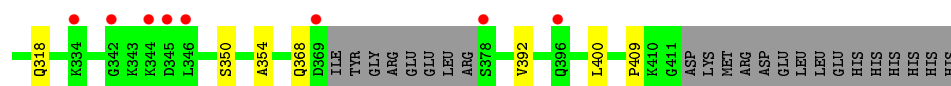


• Molecule 1: HSP47



• Molecule 1: HSP47





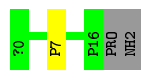
- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain E: 89% 5% 5%



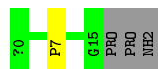
- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain F: 84% 5% 11%



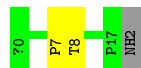
- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain G: 79% 5% 16%



- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain H: 84% 11% 5%



- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain I: 79% 11% 11%



- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain J: 74% 11% 16%



- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain M: 95% 5%



- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain N:  95% 5%




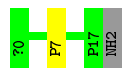
- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain O:  95% 5%



- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain R:  89% 5% 5%




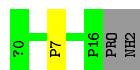
- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain S:  95% 5%



- Molecule 2: COLLAGEN MODEL PEPTIDE 18-T8R11

Chain T:  84% 5% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.71Å 104.91Å 171.84Å 90.00° 103.71° 90.00°	Depositor
Resolution (Å)	49.16 – 2.55 49.16 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.16-2.55) 98.1 (49.16-2.55)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.195 , 0.218 0.217 , 0.236	Depositor DCC
$R_{free}$ test set	1779 reflections (1.57%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	7 of 113420 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24911	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0277e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: SIN, ACE

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	0.43	0/3041	0.69	0/4101
1	B	0.43	0/2913	0.69	0/3928
1	C	0.43	0/3021	0.70	0/4073
1	D	0.44	0/2952	0.69	0/3980
1	K	0.44	0/3015	0.68	0/4063
1	L	0.44	0/2960	0.70	0/3990
1	P	0.43	0/2998	0.70	0/4042
1	Q	0.45	0/2930	0.70	0/3951
2	E	0.49	0/118	0.47	0/168
2	F	0.42	0/110	0.43	0/156
2	G	0.39	0/102	0.45	0/144
2	H	0.46	0/118	0.50	0/168
2	I	0.43	0/110	0.39	0/156
2	J	0.42	0/102	0.50	0/144
2	M	0.45	0/118	0.47	0/168
2	N	0.46	0/118	0.44	0/168
2	O	0.45	0/118	0.47	0/168
2	R	0.47	0/118	0.46	0/168
2	S	0.50	0/118	0.40	0/168
2	T	0.43	0/110	0.43	0/156
All	All	0.44	0/25190	0.68	0/34060

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 ⓘ

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	2981	0	2995	16	0
1	B	2855	0	2880	17	0
1	C	2961	0	2982	17	0
1	D	2894	0	2918	13	0
1	K	2955	0	2982	11	0
1	L	2902	0	2926	24	0
1	P	2938	0	2953	13	0
1	Q	2872	0	2895	11	0
2	E	111	0	108	1	0
2	F	104	0	101	1	0
2	G	97	0	94	1	0
2	H	111	0	108	3	0
2	I	104	0	101	2	0
2	J	97	0	94	2	0
2	M	111	0	108	0	0
2	N	111	0	108	0	0
2	O	111	0	108	0	0
2	R	111	0	108	2	0
2	S	111	0	108	0	0
2	T	104	0	101	1	0
3	A	8	0	4	1	0
3	C	8	0	4	1	0
3	K	8	0	4	0	0
3	P	8	4	4	0	0
3	Q	8	4	4	0	0
4	A	23	0	0	0	0
4	B	21	0	0	3	0
4	C	33	0	0	0	0
4	D	37	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	I	2	0	0	0	0
4	K	24	0	0	0	0
4	L	27	0	0	1	0
4	N	3	0	0	0	0
4	P	18	0	0	0	0
4	Q	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	1	0	0	0	0
4	S	2	0	0	0	0
4	T	1	0	0	0	0
All	All	24903	8	24798	123	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 2.

The worst 5 of 123 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:127:THR:HG23	1:C:207:LYS:HB3	1.48	0.94
1:A:126:VAL:HG12	1:A:209:HIS:H	1.46	0.79
1:C:374:GLU:HG3	1:C:376:LEU:HB2	1.63	0.78
1:D:42:THR:HG22	1:D:46:ARG:HH12	1.53	0.73
1:B:218:MET:CE	4:B:2008:HOH:O	2.40	0.69

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	376/392 (96%)	363 (96%)	12 (3%)	1 (0%)	46	66
1	B	358/392 (91%)	350 (98%)	8 (2%)	0	100	100
1	C	372/392 (95%)	358 (96%)	14 (4%)	0	100	100
1	D	362/392 (92%)	351 (97%)	11 (3%)	0	100	100
1	K	370/392 (94%)	360 (97%)	10 (3%)	0	100	100
1	L	363/392 (93%)	348 (96%)	13 (4%)	2 (1%)	30	48
1	P	369/392 (94%)	359 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	359/392 (92%)	348 (97%)	10 (3%)	1 (0%)	46	66
2	E	16/19 (84%)	16 (100%)	0	0	100	100
2	F	15/19 (79%)	15 (100%)	0	0	100	100
2	G	14/19 (74%)	14 (100%)	0	0	100	100
2	H	16/19 (84%)	16 (100%)	0	0	100	100
2	I	15/19 (79%)	15 (100%)	0	0	100	100
2	J	14/19 (74%)	14 (100%)	0	0	100	100
2	M	16/19 (84%)	16 (100%)	0	0	100	100
2	N	16/19 (84%)	16 (100%)	0	0	100	100
2	O	16/19 (84%)	16 (100%)	0	0	100	100
2	R	16/19 (84%)	16 (100%)	0	0	100	100
2	S	16/19 (84%)	16 (100%)	0	0	100	100
2	T	15/19 (79%)	15 (100%)	0	0	100	100
All	All	3114/3364 (93%)	3022 (97%)	88 (3%)	4 (0%)	56	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	103	ARG
1	L	105	GLU
1	A	374	GLU
1	Q	368	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	
1	A	320/337 (95%)	309 (97%)	11 (3%)	44	70
1	B	308/337 (91%)	297 (96%)	11 (4%)	42	67
1	C	319/337 (95%)	311 (98%)	8 (2%)	55	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	313/337 (93%)	300 (96%)	13 (4%)	36	60
1	K	320/337 (95%)	308 (96%)	12 (4%)	40	65
1	L	314/337 (93%)	304 (97%)	10 (3%)	46	72
1	P	317/337 (94%)	304 (96%)	13 (4%)	37	61
1	Q	311/337 (92%)	296 (95%)	15 (5%)	31	53
2	E	12/12 (100%)	12 (100%)	0	100	100
2	F	11/12 (92%)	11 (100%)	0	100	100
2	G	10/12 (83%)	10 (100%)	0	100	100
2	H	12/12 (100%)	12 (100%)	0	100	100
2	I	11/12 (92%)	11 (100%)	0	100	100
2	J	10/12 (83%)	10 (100%)	0	100	100
2	M	12/12 (100%)	12 (100%)	0	100	100
2	N	12/12 (100%)	12 (100%)	0	100	100
2	O	12/12 (100%)	12 (100%)	0	100	100
2	R	12/12 (100%)	12 (100%)	0	100	100
2	S	12/12 (100%)	12 (100%)	0	100	100
2	T	11/12 (92%)	11 (100%)	0	100	100
All	All	2659/2840 (94%)	2566 (96%)	93 (4%)	43	68

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	330	ILE
1	K	299	LYS
1	Q	260	LEU
1	K	42	THR
1	K	195	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	108	HIS
1	Q	318	GLN
1	L	318	GLN
1	D	318	GLN

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Mol	Chain	Res	Type
1	P	108	HIS

### 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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SIN	A	1421	-	1,7,7	0.21	0	2,8,8	0.77	0
3	SIN	C	1418	-	1,7,7	0.02	0	2,8,8	0.94	0
3	SIN	K	1415	-	1,7,7	0.23	0	2,8,8	0.79	0
3	SIN	P	1416	-	1,7,7	0.16	0	2,8,8	0.73	0
3	SIN	Q	1412	-	1,7,7	0.01	0	2,8,8	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIN	A	1421	-	-	0/1/5/5	0/0/0/0
3	SIN	C	1418	-	-	0/1/5/5	0/0/0/0
3	SIN	K	1415	-	-	0/1/5/5	0/0/0/0
3	SIN	P	1416	-	-	0/1/5/5	0/0/0/0
3	SIN	Q	1412	-	-	0/1/5/5	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1421	SIN	1	0
3	C	1418	SIN	1	0

## 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, 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	A	380/392 (96%)	0.44	29 (7%) 17 19	28, 57, 105, 133	0
1	B	364/392 (92%)	0.29	18 (4%) 33 39	22, 54, 107, 147	0
1	C	376/392 (95%)	0.48	38 (10%) 9 10	24, 57, 118, 148	0
1	D	368/392 (93%)	0.31	23 (6%) 23 27	22, 49, 102, 133	0
1	K	374/392 (95%)	0.27	17 (4%) 37 43	25, 53, 96, 125	0
1	L	369/392 (94%)	0.47	30 (8%) 15 16	22, 59, 119, 140	0
1	P	373/392 (95%)	0.36	18 (4%) 34 40	26, 59, 103, 131	0
1	Q	365/392 (93%)	0.19	13 (3%) 46 53	24, 50, 98, 125	0
2	E	17/19 (89%)	-0.13	0 100 100	24, 30, 66, 75	0
2	F	16/19 (84%)	-0.07	0 100 100	27, 35, 59, 68	0
2	G	15/19 (78%)	-0.26	0 100 100	26, 31, 56, 91	0
2	H	17/19 (89%)	-0.19	0 100 100	21, 29, 65, 76	0
2	I	16/19 (84%)	-0.22	0 100 100	22, 32, 63, 71	0
2	J	15/19 (78%)	-0.06	0 100 100	19, 30, 57, 90	0
2	M	17/19 (89%)	-0.12	0 100 100	23, 31, 68, 78	0
2	N	17/19 (89%)	-0.01	0 100 100	27, 32, 71, 78	0
2	O	17/19 (89%)	-0.17	0 100 100	24, 31, 87, 100	0
2	R	17/19 (89%)	0.00	0 100 100	26, 32, 61, 67	0
2	S	17/19 (89%)	0.17	0 100 100	29, 34, 64, 76	0
2	T	16/19 (84%)	0.10	0 100 100	28, 33, 65, 92	0
All	All	3166/3364 (94%)	0.32	186 (5%) 26 30	19, 53, 106, 148	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	PHE	6.7
1	C	344	LYS	6.2
1	P	344	LYS	6.1
1	C	346	LEU	5.9
1	L	39	LYS	5.9

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SIN	C	1418	8/8	0.73	0.20	2.63	55,58,62,64	0
3	SIN	A	1421	8/8	0.76	0.20	2.56	59,62,64,65	0
3	SIN	K	1415	8/8	0.78	0.20	2.04	56,60,63,64	0
3	SIN	P	1416	8/8	0.73	0.20	1.85	71,73,76,77	0
3	SIN	Q	1412	8/8	0.88	0.14	-0.07	50,60,68,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.