



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1Y4S  
Title : Conformation rearrangement of heat shock protein 90 upon ADP binding  
Authors : Huai, Q.; Wang, H.; Liu, Y.; Kim, H.; Toft, D.; Ke, H.  
Deposited on : 2004-12-01  
Resolution : 2.90 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

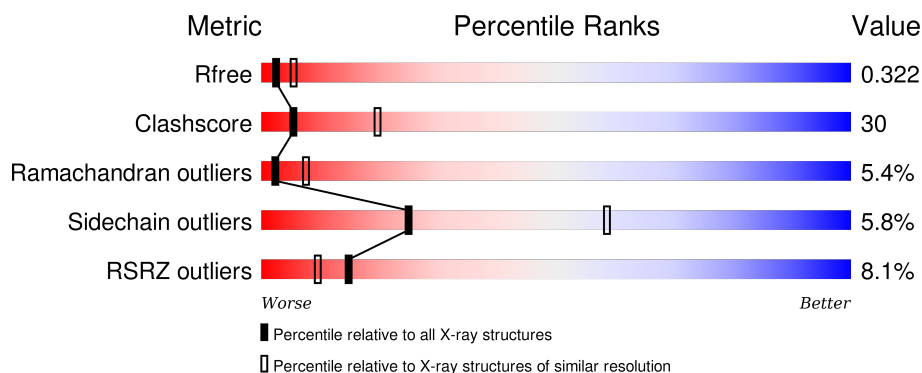
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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  $\geq 3$ , 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	559	<div> <div>8%</div> <div>43%</div> <div>36%</div> <div>6%</div> <div>15%</div> </div>
1	B	559	<div> <div>6%</div> <div>37%</div> <div>43%</div> <div>•</div> <div>15%</div> </div>

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
2	MG	A	703	-	-	-	X
2	MG	B	704	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7784 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.

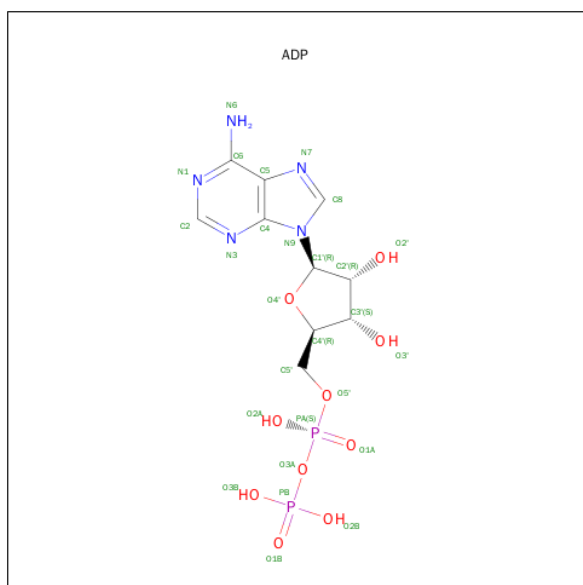
- Molecule 1 is a protein called Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			
1	B	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



ASP	ARG	VAL	LYS	ALA	LEU	LEU	GLY	GLU	ARG	VAL	LYS	ASP	VAL	ARG	LEU	THR	HIS	ARG	LEU	THR	ASP	THR	PRO	ALA	ILE	VAL	SER	THR	ASP	ALA	ASP	GLU	GLU	MET	SER	THR	GLN	SER	GLN	LEU	MET	ALA	LYS	LEU	PHE	ALA	ALA	GLY	GLN					
R446	L447	E448	L449	L450	R451	G452	I455	E456	L459	L460	R463	I464	E465	W466	L472	T473	E474	F475	D476	G477	K478	P479	S482	V483	SER	LYS	VAL	ASP	GLU	THR	GLN	SER	GLU	LEU	LEU	GLU	LYS	LEU	ALA	ASP	GLU	VAL	ASP	SER	ALA	LYS	GLU	ALA	THR	PRO	PHE	ILE		
Q372	W375	Q376	Q377	F378	G379	L380	V381	L382	K383	G384	G385	F386	A387	E388	D389	E394	A395	I396	L399	L400	R401	F402	A403	S404	T405	D408	V414	S415	D418	Y419	V420	S421	R422	N423	K424	E425	G426	Q427	K428	K429	Y432	I433	T434	A435	Y438	A441	K442	S443	S444	P445				
L299	Y300	V301	Q302	F305	I306	M307	D308	E311	Q312	F313	M314	P315	N316	Y317	L318	R319	F320	V321	R322	G323	L324	I325	D326	L330	P331	L332	N333	V334	I338	Q340	D341	S342	T345	R346	N347	L348	K354	R355	Q358	N359	L360	E361	K362	L363	A364	K365	D366	D367	K370	Y371				
K226	I227	N228	K229	A230	Q231	A232	L233	W234	T235	K238	S239	E240	D243	E244	E245	Y246	K247	E248	F249	Y250	K251	H252	L253	D256	F257	N258	D259	P260	L261	T262	H265	E269	G270	K271	Q272	S276	L277	L278	Y279	I280	P281	S282	P285	W286	D287	M288	R291	D292	L297	K298				
V152	F153	W154	E155	S156	G160	E161	Y162	T163	V164	A165	D166	I167	T168	D171	R172	G173	T174	E175	I176	T177	L178	H179	L180	L188	D189	D190	W191	R192	V193	R194	S195	I196	I197	S198	D202	H203	I204	A205	L206	P207	V208	E209	I210	E211	K216	D217	G218	E219	T220	V221	L222	S223	W224	E225
N81	G82	V83	G84	M85	T86	E89	L94	G95	T96	I97	A98	K99	S100	G101	T102	K103	S104	F105	L106	E107	S108	LEU	GLY	SER	ASP	GLN	ALA	LYS	ASP	S117	Q118	L119	I120	G121	Q122	F123	G124	V125	G126	F127	Y128	V133	A134	V139	R140	T141	R142	A143	E146	K147	P148	E149		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.50 Å   84.18 Å   212.89 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.90 78.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 88.4 (78.28-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.82 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.269   ,   0.314 0.275   ,   0.322	Depositor DCC
$R_{free}$ test set	2728 reflections (9.72%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 53882 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	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 56.84 % 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 2.5801e-05. 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.52	0/3941	0.78	3/5314 (0.1%)
1	B	0.48	0/3941	0.71	2/5314 (0.0%)
All	All	0.50	0/7882	0.75	5/10628 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLY	N-CA-C	-8.81	91.07	113.10
1	B	426	GLY	N-CA-C	-6.12	97.81	113.10
1	A	123	PHE	N-CA-C	5.89	126.89	111.00
1	B	447	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	400	LEU	CA-CB-CG	5.46	127.87	115.30

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	3864	0	3786	215	0
1	B	3864	0	3786	245	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	0	0
3	B	27	0	12	0	0
All	All	7784	0	7596	460	1

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 30.

The worst 5 of 460 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:B:402:PHE:HD1	1:B:460:LEU:HD21	1.11	1.14
1:A:463:ARG:H	1:A:463:ARG:HD2	1.17	1.06
1:B:402:PHE:CD1	1:B:460:LEU:HD21	1.92	1.02
1:B:2:LYS:H	1:B:2:LYS:HD3	1.25	0.98
1:A:242:THR:HG22	1:A:244:GLU:H	1.27	0.96

All (1) 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:B:338:ILE:CD1	1:B:338:ILE:CD1[2_655]	2.15	0.05

## 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	471/559 (84%)	368 (78%)	78 (17%)	25 (5%)	2	8
1	B	471/559 (84%)	366 (78%)	79 (17%)	26 (6%)	2	7
All	All	942/1118 (84%)	734 (78%)	157 (17%)	51 (5%)	2	7

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	125	VAL
1	A	288	MET
1	A	290	ASN
1	A	292	ASP

### 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	419/488 (86%)	395 (94%)	24 (6%)	25	59
1	B	419/488 (86%)	394 (94%)	25 (6%)	24	57
All	All	838/976 (86%)	789 (94%)	49 (6%)	25	58

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	PRO
1	B	161	GLU
1	B	408	ASP
1	B	2	LYS
1	B	163	THR

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

Mol	Chain	Res	Type
1	A	481	GLN
1	B	4	GLN
1	B	272	GLN
1	A	427	GLN
1	B	350	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ADP	A	701	2	22,29,29	0.73	0	27,45,45	1.52	2 (7%)
3	ADP	B	702	2	22,29,29	0.77	0	27,45,45	1.46	2 (7%)

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	ADP	A	701	2	-	0/12/32/32	0/3/3/3
3	ADP	B	702	2	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ADP	PA-O3A-PB	-6.93	109.44	132.67
3	B	702	ADP	PA-O3A-PB	-6.54	110.75	132.67
3	A	701	ADP	O3A-PA-O5'	2.12	108.57	102.94
3	B	702	ADP	O3A-PA-O5'	2.53	109.66	102.94

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

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	A	475/559 (84%)	0.60	42 (8%) 12 8	9, 58, 100, 100	0
1	B	475/559 (84%)	0.55	35 (7%) 17 11	33, 70, 98, 100	0
All	All	950/1118 (84%)	0.58	77 (8%) 15 9	9, 65, 100, 100	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	SER	13.5
1	A	108	SER	8.3
1	A	107	GLU	7.7
1	B	105	PHE	7.4
1	A	118	GLN	6.8

### 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](#)

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( $\text{\AA}^2$ )	Q<0.9
2	MG	B	704	1/1	0.94	0.31	7.78	28,28,28,28	0
2	MG	A	703	1/1	0.99	0.32	4.13	26,26,26,26	0
3	ADP	A	701	27/27	0.96	0.19	-0.48	22,26,28,29	0
3	ADP	B	702	27/27	0.96	0.16	-1.43	27,35,38,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.