



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1Y4U
Title : Conformation rearrangement of heat shock protein 90 upon ADP binding
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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
A user guide is available at
<http://wwpdb.org/validation/2016/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
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

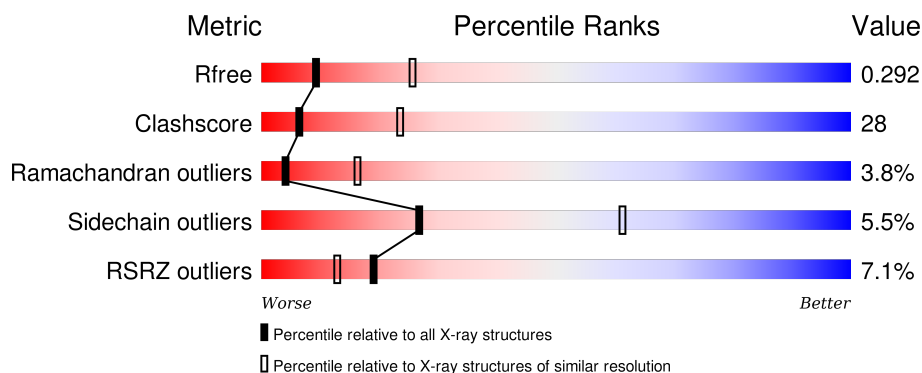
1 Overall quality at a glance

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 ≥ 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	
1	B	559	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7536 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	472	Total	C	N	O	S	0	0	0
			3837	2421	660	746	10			
1	B	454	Total	C	N	O	S	0	0	0
			3699	2338	634	718	9			

PRO	PHE	ILE	ASP	ARG	VAL	LYS	ALA	LEU	GLY	GLU	ARG	VAL	LYS	ASP	VAL	ARG	LEU	THR	HIS	ANG	LEU	THR	ASP	THR	PRO	ALA	ILE	VAL	SER	THR	ASP	ALA	ASP	GLU	MET	SER	THR	GLN	THR	MET	ALA	LYS	LEU	PHE	ALA	ALA	GLY	GLN	G158	E159	I167	T168	K169	E170	D171	R172	G173	I176	R181	F187	W191	R192	V193	R194	S195	I196	I197	S198	K199	Y200	L204	A205	L206	P207	V208	E209	I210	E211	K212	R213	E214	E215	K216	D217	G218	E219	T220	E225	K226	I227	N228	K229	A230	Q231	A232	L233	W234	T235	R236	N237	K238
M423	Q427	I430	Y431	Y432	I433	T434	A435	D436	S437	Y438	A439	A440	A441	K442	S443	S444	P445	H446	L447	I464	M468	M469	L472	K478	S482	V483	S484	K485	V486	D487	E488	S489	LEU	GLU	LYS	LEU	LYS	LEU	PHE	ALA	GLU	VAL	ASP	GLY	GLN	S239	E240	I241	T242	D243	E244	E245	F249	Y250	K251	H252	I253	A254	F257	N258	D259	T262	W263	G270	K271	Q272	E273	Y274	L278	P281	W286	D287	N288	R291	D292	R293	K294	H295	L299	Y300	V301	F305	I306	K307	D308	Q312	N316	R319	F320	V321	R322	G323									

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.01Å 158.01Å 117.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 94.04 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 83.5 (94.04-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.82Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.295 0.233 , 0.292	Depositor DCC
R_{free} test set	3001 reflections (9.96%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 32234 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7536	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.73	4/3913 (0.1%)	0.98	9/5277 (0.2%)
1	B	0.47	0/3774	0.72	1/5095 (0.0%)
All	All	0.62	4/7687 (0.1%)	0.86	10/10372 (0.1%)

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	A	0	4
1	B	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	HIS	C-O	29.99	1.80	1.23
1	A	8	GLY	C-N	-16.40	0.96	1.34
1	A	8	GLY	C-O	11.09	1.41	1.23
1	A	10	GLN	C-N	-7.64	1.16	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	GLY	O-C-N	-30.14	74.47	122.70
1	A	293	HIS	O-C-N	-29.82	75.00	122.70
1	A	8	GLY	CA-C-N	18.88	158.73	117.20
1	A	8	GLY	C-N-CA	18.75	168.57	121.70
1	A	8	GLY	CA-C-O	-9.09	104.25	120.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ASP	Mainchain
1	A	293	HIS	Mainchain
1	A	8	GLY	Mainchain,Peptide
1	B	371	TYR	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	A	3837	0	3753	242	0
1	B	3699	0	3612	196	0
All	All	7536	0	7365	411	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 28.

The worst 5 of 411 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:A:293:HIS:C	1:A:293:HIS:O	1.80	1.20
1:A:10:GLN:O	1:A:11:SER:HB2	1.49	1.13
1:B:291:ARG:HD2	1:B:291:ARG:H	1.16	1.04
1:A:242:THR:HG22	1:A:244:GLU:H	1.24	1.01
1:A:293:HIS:O	1:A:294:LYS:N	1.94	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	468/559 (84%)	386 (82%)	60 (13%)	22 (5%)	3	11
1	B	450/559 (80%)	397 (88%)	40 (9%)	13 (3%)	6	23
All	All	918/1118 (82%)	783 (85%)	100 (11%)	35 (4%)	4	16

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	LYS
1	A	15	GLN
1	A	17	LEU
1	A	293	HIS

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	416/488 (85%)	395 (95%)	21 (5%)	30	65
1	B	401/488 (82%)	377 (94%)	24 (6%)	24	57
All	All	817/976 (84%)	772 (94%)	45 (6%)	27	61

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	473	THR
1	B	170	GLU
1	B	380	LEU
1	B	58	GLU
1	B	171	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	GLN
1	B	93	HIS
1	B	283	GLN
1	A	412	GLN
1	B	81	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](#)

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(Å ²)	Q<0.9
1	A	472/559 (84%)	0.49	37 (7%)	16 10	34, 66, 101, 101	0
1	B	454/559 (81%)	0.43	29 (6%)	23 16	19, 46, 99, 101	0
All	All	926/1118 (82%)	0.46	66 (7%)	19 13	19, 57, 101, 101	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	12.3
1	A	488	GLU	9.8
1	B	487	ASP	9.7
1	A	489	SER	8.8
1	A	12	GLU	8.7

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.