



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:51 AM GMT

PDB ID : 3Q6M  
Title : Crystal Structure of Human MC-HSP90 in C2221 Space Group  
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Deposited on : 2011-01-03  
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) : 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

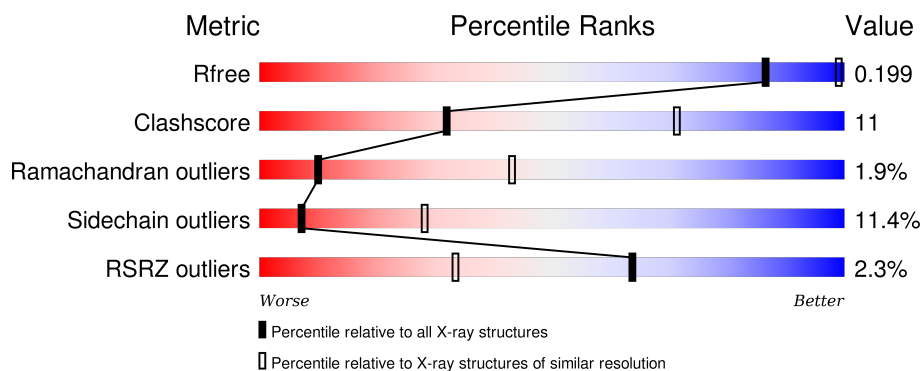
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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.

Mol	Chain	Length	Quality of chain
1	A	448	<div> <div>2%</div> <div>59% 19% 5% 17%</div> </div>
1	B	448	<div> <div>%</div> <div>63% 16% 5% 17%</div> </div>
1	C	448	<div> <div>3%</div> <div>59% 19% • 18%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9345 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			3069	1954	518	582	15			
1	B	374	Total	C	N	O	S	0	0	0
			3085	1964	520	586	15			
1	C	369	Total	C	N	O	S	0	0	0
			3043	1939	512	577	15			

There are 24 discrepancies between the modelled and reference sequences:

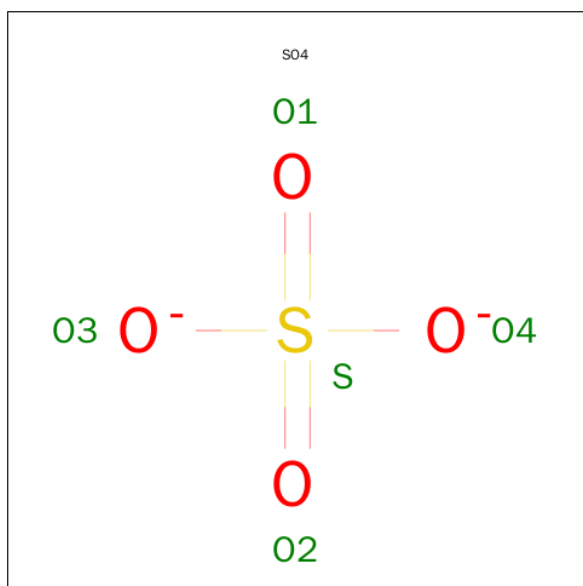
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	-	EXPRESSION TAG	UNP P07900
A	292	ALA	-	EXPRESSION TAG	UNP P07900
A	733	HIS	-	EXPRESSION TAG	UNP P07900
A	734	HIS	-	EXPRESSION TAG	UNP P07900
A	735	HIS	-	EXPRESSION TAG	UNP P07900
A	736	HIS	-	EXPRESSION TAG	UNP P07900
A	737	HIS	-	EXPRESSION TAG	UNP P07900
A	738	HIS	-	EXPRESSION TAG	UNP P07900
B	291	ALA	-	EXPRESSION TAG	UNP P07900
B	292	ALA	-	EXPRESSION TAG	UNP P07900
B	733	HIS	-	EXPRESSION TAG	UNP P07900
B	734	HIS	-	EXPRESSION TAG	UNP P07900
B	735	HIS	-	EXPRESSION TAG	UNP P07900
B	736	HIS	-	EXPRESSION TAG	UNP P07900
B	737	HIS	-	EXPRESSION TAG	UNP P07900
B	738	HIS	-	EXPRESSION TAG	UNP P07900
C	291	ALA	-	EXPRESSION TAG	UNP P07900
C	292	ALA	-	EXPRESSION TAG	UNP P07900
C	733	HIS	-	EXPRESSION TAG	UNP P07900
C	734	HIS	-	EXPRESSION TAG	UNP P07900
C	735	HIS	-	EXPRESSION TAG	UNP P07900
C	736	HIS	-	EXPRESSION TAG	UNP P07900
C	737	HIS	-	EXPRESSION TAG	UNP P07900

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Chain	Residue	Modelled	Actual	Comment	Reference
C	738	HIS	-	EXPRESSION TAG	UNP P07900

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	53	Total	O	0	0
			53	53		
3	C	36	Total	O	0	0
			36	36		

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 ( $\text{RSRZ} > 2$ ). 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.

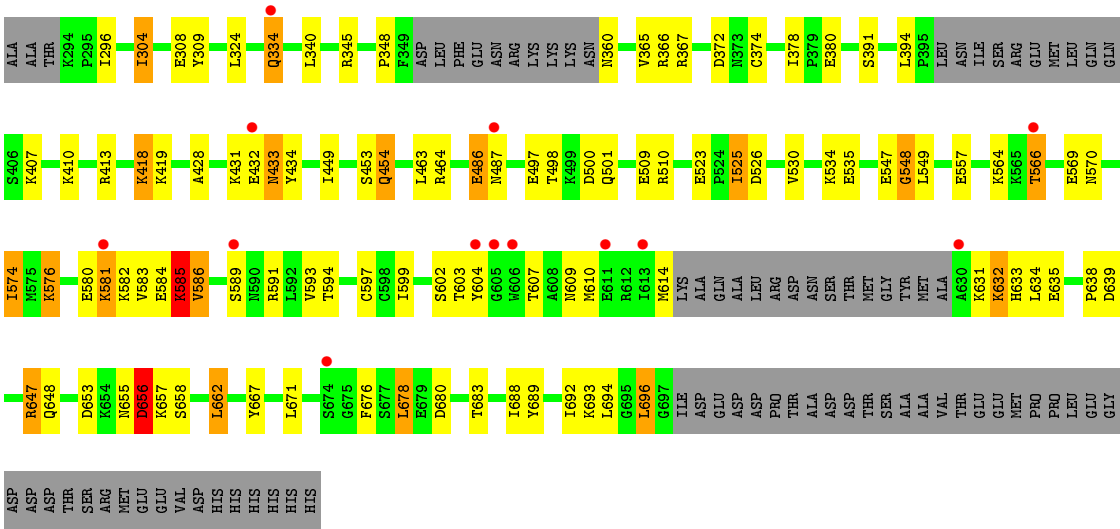
- [illegible]

- Chain B:

63% 16% 5% 17%

Index	Amino Acid	Category
1	ALA	Non-polar
2	ALA	Non-polar
3	THR	Polar
4	P294	Polar
5	P295	Polar
6	L296	Polar
7	M297	Polar
8	I304	Non-polar
9	E308	Polar
10	Y309	Polar
11	L316	Non-polar
12	L340	Non-polar
13	R346	Basic
14	F349	Aromatic
15	ASP	Polar
16	ASP	Polar
17	PHE	Aromatic
18	GLU	Polar
19	ASN	Polar
20	ARG	Polar
21	LVS	Non-polar
22	LVS	Non-polar
23	R359	Basic
24	R362	Basic
25	R367	Basic
26	R373	Basic
27	C374	Aromatic
28	E375	Polar
29	E376	Polar
30	L377	Non-polar
31	L378	Non-polar
32	G387	Polar
33	V388	Non-polar
34	E392	Polar
35	D393	Polar
36	L394	Non-polar
37	P395	Polar
38	LEU	Non-polar
39	ASN	Polar
40	ILE	Non-polar
41	SER	Polar
42	ARG	Polar
43	GLU	Polar
44	MET	Polar
45	LEU	Non-polar
46	GLN	Polar
47	Q405	Polar
48	R406	Basic

- Chain C:  3% 59% 19% 18%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.70Å 304.55Å 87.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-3.00) 95.0 (29.84-3.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.209 , 0.252 0.204 , 0.199	Depositor DCC
$R_{free}$ test set	2184 reflections (5.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 76.1	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	0 of 43622 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9345	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: SO4

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	0.62	0/3120	0.69	0/4188
1	B	0.66	0/3136	0.71	1/4210 (0.0%)
1	C	0.57	0/3094	0.65	1/4154 (0.0%)
All	All	0.61	0/9350	0.68	2/12552 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	646	LEU	CA-CB-CG	7.56	132.69	115.30
1	C	696	LEU	CA-CB-CG	5.52	128.00	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	3069	0	3108	72	0
1	B	3085	0	3123	70	0
1	C	3043	0	3081	64	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	0	1	0
3	B	53	0	0	0	0
3	C	36	0	0	1	0
All	All	9345	0	9312	197	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 11.

The worst 5 of 197 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:367:ARG:HG3	1:B:367:ARG:HH11	1.15	1.03
1:C:607:THR:HG22	1:C:610:MET:HG3	1.43	0.99
1:B:410:LYS:HE3	1:B:414:LYS:HE3	1.44	0.97
1:C:525:ILE:H	1:C:525:ILE:HD12	1.32	0.94
1:A:656:ASP:HB3	1:A:659:VAL:HG23	1.48	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	
1	A	364/448 (81%)	344 (94%)	15 (4%)	5 (1%)	14	51
1	B	366/448 (82%)	335 (92%)	26 (7%)	5 (1%)	14	51
1	C	361/448 (81%)	323 (90%)	27 (8%)	11 (3%)	5	29
All	All	1091/1344 (81%)	1002 (92%)	68 (6%)	21 (2%)	10	43

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	580	GLU
1	B	376	GLU
1	C	432	GLU
1	A	429	GLU
1	A	696	LEU

### 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	346/412 (84%)	305 (88%)	41 (12%)	6	26
1	B	348/412 (84%)	309 (89%)	39 (11%)	7	29
1	C	343/412 (83%)	305 (89%)	38 (11%)	8	29
All	All	1037/1236 (84%)	919 (89%)	118 (11%)	7	28

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	435	LYS
1	B	578	ILE
1	C	614	MET
1	B	443	LYS
1	B	535	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	487	ASN
1	B	501	GLN
1	C	487	ASN
1	B	450	HIS
1	B	454	GLN

### 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 ⓘ

3 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	$\# Z  > 2$
2	SO4	A	1	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	B	2	-	4,4,4	0.23	0	6,6,6	0.39	0
2	SO4	C	3	-	4,4,4	0.19	0	6,6,6	0.22	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
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3	-	-	0/0/0/0	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.

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	372/448 (83%)	-0.13	8 (2%) 65 35	67, 94, 136, 185	0
1	B	374/448 (83%)	-0.18	5 (1%) 79 53	61, 89, 143, 174	0
1	C	369/448 (82%)	-0.01	13 (3%) 48 21	69, 114, 187, 222	0
All	All	1115/1344 (82%)	-0.10	26 (2%) 64 33	61, 98, 161, 222	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	606	TRP	4.4
1	C	630	ALA	4.4
1	A	395	PRO	4.3
1	C	604	TYR	4.0
1	A	559	LYS	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](#)

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	SO4	A	1	5/5	0.92	0.14	-	127,128,128,129	0
2	SO4	B	2	5/5	0.90	0.19	-	120,121,122,123	0
2	SO4	C	3	5/5	0.70	0.32	-	164,165,165,165	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.