



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 AM GMT

PDB ID : 2CCU  
Title : HUMAN HSP90 WITH 4-CHLORO-6-(4-(4-METHANESULPHONYL-B  
ENZYL)-PIERAZIN-1-YL)-1H-PYRAZOL-3-YL)-BENZENE-1,3-DIOL  
Authors : Barril, X.; Beswick, M.C.; Collier, A.; Drysdale, M.J.; Dymock, B.W.; Fink,  
A.; Grant, K.; Howes, R.; Jordan, A.M.; Massey, A.; Surgenor, A.; Wayne, J.;  
Workman, P.; Wright, L.  
Deposited on : 2006-01-18  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

---

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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



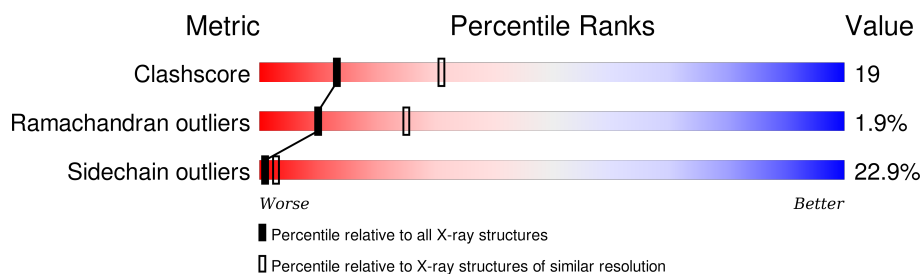
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	236	



## 2 Entry composition [i](#)

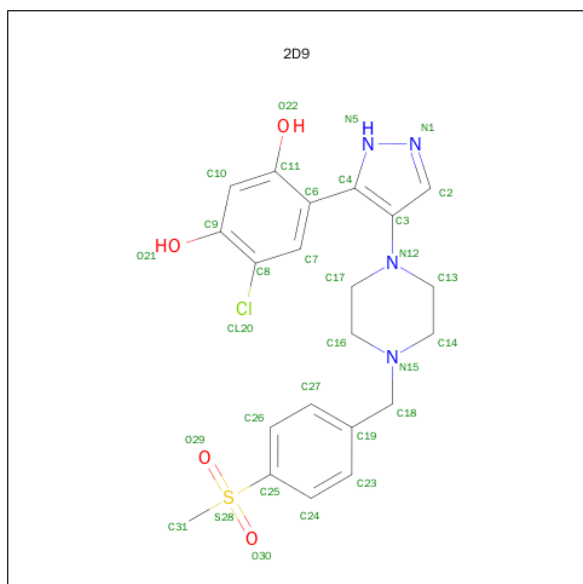
There are 3 unique types of molecules in this entry. The entry contains 1726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	209	Total	C	N	O	S	0	0	1
			1621	1029	267	320	5			

- Molecule 2 is 4-CHLORO-6-(4-{4-[4-(METHYLSULFONYL)BENZYL]PIPERAZIN-1-YL}-1H-PYRAZOL-5-YL)BENZENE-1,3-DIOL (three-letter code: 2D9) (formula: C<sub>21</sub>H<sub>23</sub>ClN<sub>4</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			31	21	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		



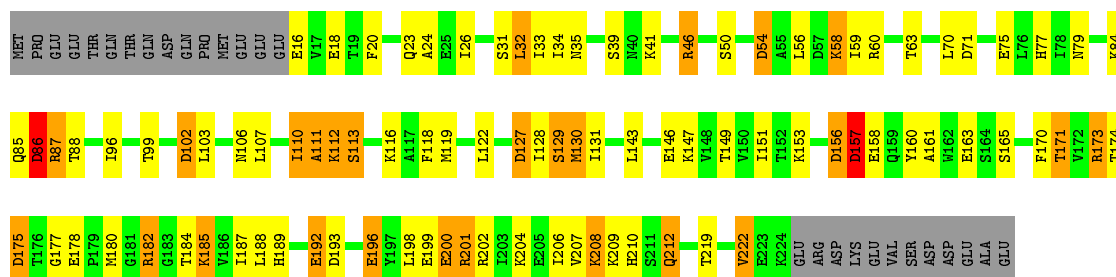
### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

#### • Molecule 1: HEAT SHOCK PROTEIN HSP-90 ALPHA

Chain A: 





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.47Å 88.87Å 99.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (30.00-2.70)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.237 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2D9

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	0.95	0/1647	1.12	9/2226 (0.4%)

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	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	CB-CG-OD2	7.53	125.07	118.30
1	A	54	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	102	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	71	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	157	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	86	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	193	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	111	ALA	N-CA-C	5.13	124.85	111.00
1	A	127	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	GLU	Peptide



## 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	1621	0	1604	62	0
2	A	31	0	22	2	0
3	A	74	0	0	13	0
All	All	1726	0	1626	62	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 19.

All (62) 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:59:ILE:O	1:A:63:THR:HG23	1.51	1.07
1:A:201:ARG:HH11	1:A:201:ARG:HG2	1.43	0.83
1:A:23:GLN:HB2	1:A:26:ILE:HD13	1.65	0.78
1:A:201:ARG:NH1	1:A:201:ARG:HG2	2.06	0.70
1:A:32:LEU:HD23	1:A:32:LEU:C	2.13	0.69
1:A:171:THR:CG2	3:A:2053:HOH:O	2.40	0.69
1:A:189:HIS:HB3	3:A:2049:HOH:O	1.92	0.68
1:A:147:LYS:HE2	1:A:163:GLU:OE2	1.94	0.68
1:A:46:ARG:HG3	1:A:210:HIS:HB3	1.77	0.67
1:A:106:ASN:ND2	3:A:2038:HOH:O	2.29	0.66
1:A:127:ASP:O	1:A:130:MET:HG2	1.95	0.65
1:A:26:ILE:HD12	1:A:26:ILE:N	2.15	0.62
1:A:200:GLU:HG3	1:A:204:LYS:HD2	1.82	0.62
1:A:85:GLN:HB3	3:A:2028:HOH:O	1.99	0.62
1:A:63:THR:HG21	1:A:70:LEU:HG	1.81	0.62
1:A:86:ASP:OD1	1:A:86:ASP:N	2.30	0.61
1:A:173:ARG:HD3	3:A:2058:HOH:O	1.99	0.60
1:A:112:LYS:HD3	1:A:113:SER:H	1.65	0.60
1:A:87:ARG:HG3	3:A:2026:HOH:O	2.01	0.60
1:A:200:GLU:OE2	1:A:222:VAL:HG23	2.01	0.59
1:A:151:ILE:O	1:A:184:THR:HA	2.02	0.59
1:A:157:ASP:HB3	3:A:2051:HOH:O	2.04	0.56
1:A:160:TYR:CE1	1:A:174:THR:HG22	2.41	0.56
1:A:200:GLU:O	1:A:204:LYS:HG3	2.07	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASP:OD2	2:A:1224:2D9:H171	2.07	0.55
1:A:88:THR:HA	1:A:188:LEU:O	2.07	0.53
1:A:54:ASP:HB2	2:A:1224:2D9:H311	1.91	0.53
1:A:128:ILE:O	1:A:131:ILE:HG22	2.09	0.53
1:A:171:THR:HG21	3:A:2053:HOH:O	2.05	0.52
1:A:79:ASN:HD22	1:A:219:THR:HB	1.74	0.52
1:A:59:ILE:HD13	1:A:96:ILE:HG13	1.90	0.52
1:A:32:LEU:HD23	1:A:32:LEU:O	2.11	0.51
1:A:173:ARG:CD	3:A:2058:HOH:O	2.55	0.51
1:A:112:LYS:HD3	1:A:113:SER:N	2.25	0.51
1:A:112:LYS:CD	3:A:2042:HOH:O	2.59	0.50
1:A:180:MET:O	1:A:182:ARG:N	2.44	0.49
1:A:209:LYS:CB	3:A:2014:HOH:O	2.61	0.49
1:A:202:ARG:CZ	1:A:206:ILE:HD11	2.43	0.48
1:A:32:LEU:CD2	1:A:32:LEU:C	2.81	0.47
1:A:208:LYS:O	1:A:212:GLN:HG3	2.14	0.47
1:A:79:ASN:ND2	1:A:219:THR:HB	2.29	0.47
1:A:107:LEU:HD12	1:A:107:LEU:N	2.30	0.47
1:A:87:ARG:CG	3:A:2026:HOH:O	2.61	0.46
1:A:112:LYS:HD2	3:A:2042:HOH:O	2.15	0.45
1:A:54:ASP:OD2	1:A:58:LYS:HE3	2.17	0.45
1:A:208:LYS:C	1:A:208:LYS:HD3	2.37	0.45
1:A:33:ILE:HG23	1:A:143:LEU:HD23	1.99	0.45
1:A:196:GLU:O	1:A:199:GLU:HB2	2.17	0.44
1:A:160:TYR:HE1	1:A:174:THR:HG22	1.81	0.44
1:A:200:GLU:OE2	1:A:222:VAL:CG2	2.64	0.44
1:A:102:ASP:O	1:A:103:LEU:C	2.56	0.44
1:A:20:PHE:HB2	1:A:170:PHE:CZ	2.52	0.43
1:A:180:MET:HE1	1:A:185:LYS:HG3	2.00	0.43
1:A:127:ASP:OD2	1:A:129:SER:HB3	2.19	0.42
1:A:99:THR:HB	1:A:157:ASP:OD2	2.20	0.42
1:A:118:PHE:O	1:A:122:LEU:N	2.51	0.42
1:A:41:LYS:HE3	1:A:143:LEU:O	2.19	0.42
1:A:84:LYS:HA	1:A:198:LEU:HD13	2.00	0.42
1:A:149:THR:HB	1:A:187:ILE:HB	2.02	0.42
1:A:31:SER:O	1:A:35:ASN:HB2	2.19	0.42
1:A:161:ALA:HB2	1:A:175:ASP:HB2	2.02	0.41
1:A:110:ILE:HG13	1:A:110:ILE:H	1.66	0.41

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	207/236 (88%)	179 (86%)	24 (12%)	4 (2%)	10 25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ALA
1	A	111	ALA
1	A	192	GLU
1	A	177	GLY

### 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	175/206 (85%)	135 (77%)	40 (23%)	1 3

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	32	LEU
1	A	34	ILE
1	A	39	SER
1	A	46	ARG
1	A	50	SER
1	A	56	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	58	LYS
1	A	60	ARG
1	A	75	GLU
1	A	77	HIS
1	A	86	ASP
1	A	87	ARG
1	A	110	ILE
1	A	112	LYS
1	A	113	SER
1	A	116	LYS
1	A	119	MET
1	A	129	SER
1	A	130	MET
1	A	146	GLU
1	A	153	LYS
1	A	156	ASP
1	A	157	ASP
1	A	158	GLU
1	A	165	SER
1	A	171	THR
1	A	173	ARG
1	A	175	ASP
1	A	178	GLU
1	A	182	ARG
1	A	185	LYS
1	A	192	GLU
1	A	196	GLU
1	A	200	GLU
1	A	201	ARG
1	A	207	VAL
1	A	208	LYS
1	A	212	GLN
1	A	222	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	77	HIS
1	A	79	ASN
1	A	85	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 ⓘ

1 ligand is 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	2D9	A	1224	-	33,34,34	2.53	11 (33%)	43,50,50	2.85	17 (39%)

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	2D9	A	1224	-	-	0/12/28/28	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1224	2D9	C6-C4	-6.28	1.43	1.49
2	A	1224	2D9	N1-N5	-5.67	1.25	1.37
2	A	1224	2D9	C2-C3	-3.64	1.31	1.37
2	A	1224	2D9	C18-N15	2.20	1.51	1.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1224	2D9	C27-C26	2.25	1.42	1.38
2	A	1224	2D9	O30-S28	2.49	1.52	1.44
2	A	1224	2D9	C10-C9	2.83	1.42	1.38
2	A	1224	2D9	O21-C9	2.85	1.42	1.36
2	A	1224	2D9	C18-C19	3.20	1.57	1.51
2	A	1224	2D9	C9-C8	3.54	1.42	1.39
2	A	1224	2D9	C25-S28	6.64	1.85	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1224	2D9	C10-C9-C8	-5.24	115.38	118.27
2	A	1224	2D9	O29-S28-C31	-5.16	100.10	108.53
2	A	1224	2D9	O30-S28-C31	-3.34	103.07	108.53
2	A	1224	2D9	C24-C25-C26	-3.25	116.07	120.42
2	A	1224	2D9	O30-S28-O29	-2.64	112.22	117.73
2	A	1224	2D9	C17-N12-C3	2.10	121.30	116.42
2	A	1224	2D9	C16-C17-N12	2.23	115.05	110.63
2	A	1224	2D9	C19-C18-N15	2.47	117.95	113.16
2	A	1224	2D9	C13-C14-N15	2.67	115.40	110.63
2	A	1224	2D9	C23-C24-C25	2.93	122.71	119.48
2	A	1224	2D9	O29-S28-C25	3.00	110.94	108.31
2	A	1224	2D9	C14-N15-C16	3.03	115.47	108.90
2	A	1224	2D9	C13-N12-C17	3.17	118.25	111.59
2	A	1224	2D9	C6-C4-N5	3.93	125.78	120.71
2	A	1224	2D9	C26-C25-S28	6.04	125.53	119.59
2	A	1224	2D9	C31-S28-C25	7.50	113.76	104.68
2	A	1224	2D9	O30-S28-C25	8.22	115.50	108.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1224	2D9	2	0

## 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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.