



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:41 PM GMT

PDB ID : 1US7
Title : COMPLEX OF HSP90 AND P50
Authors : Roe, S.M.; Ali, M.M.U.; Pearl, L.H.
Deposited on : 2003-11-20
Resolution : 2.30 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
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

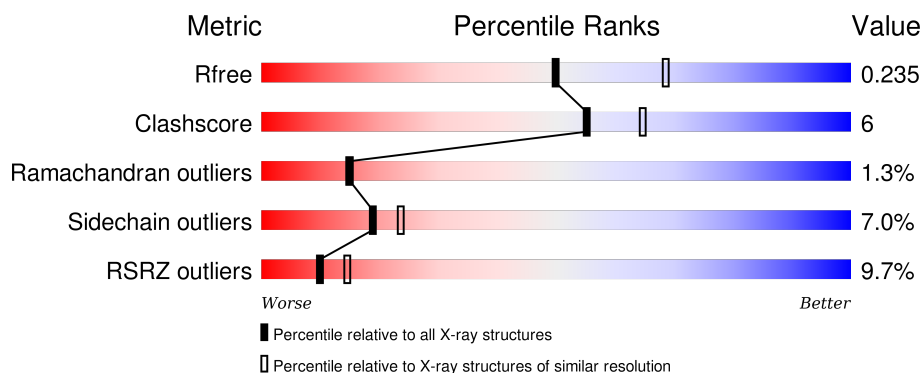
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	214	<div> <div>5%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>
2	B	265	<div> <div>11%</div> <div>51%</div> <div>15%</div> <div>6%</div> <div>•</div> <div>27%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3414 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 HSP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	1
			1639	1043	271	321	4			

- Molecule 2 is a protein called HSP90 CO-CHAPERONE CDC37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1599	1012	276	297	14			

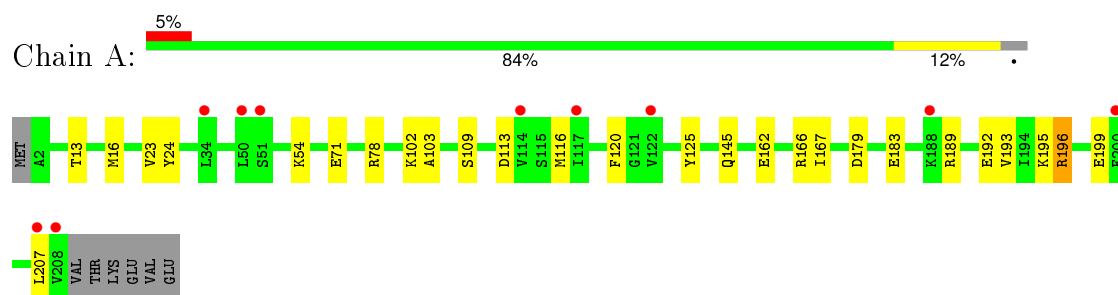
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	61	Total	O	0	0
			61	61		

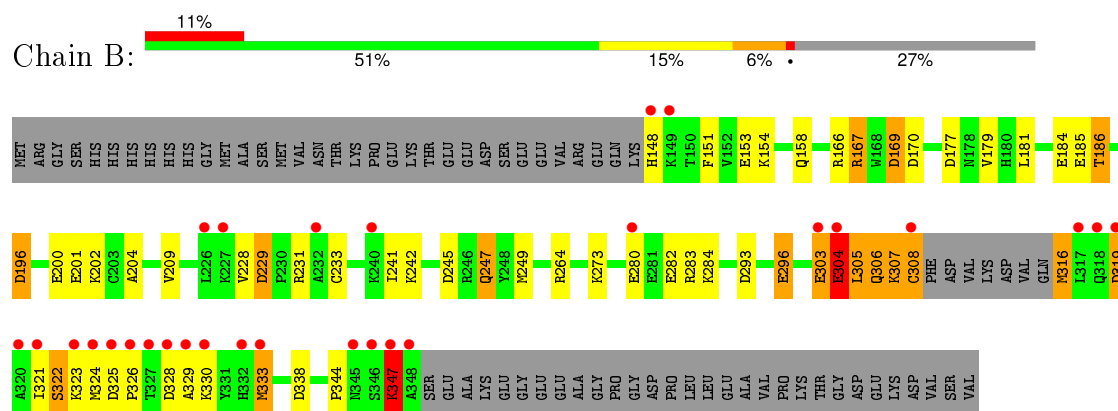
3 Residue-property plots [i](#)

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.

• Molecule 1: HEAT SHOCK PROTEIN HSP82



• Molecule 2: HSP90 CO-CHAPERONE CDC37



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.76 Å 83.76 Å 148.44 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.55 – 2.30 36.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (72.55-2.30) 96.4 (36.27-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.185 , 0.241 0.182 , 0.235	Depositor DCC
R_{free} test set	1334 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.8	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 26462 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3414	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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	1.34	4/1663 (0.2%)	1.11	4/2241 (0.2%)
2	B	1.26	2/1629 (0.1%)	1.24	18/2184 (0.8%)
All	All	1.30	6/3292 (0.2%)	1.18	22/4425 (0.5%)

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
2	B	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	MET	SD-CE	-7.76	1.34	1.77
2	B	209	VAL	CB-CG1	6.56	1.66	1.52
1	A	120	PHE	CE1-CZ	5.90	1.48	1.37
1	A	116	MET	CB-CG	5.60	1.69	1.51
1	A	125	TYR	CG-CD1	5.14	1.45	1.39
1	A	193	VAL	CB-CG1	5.10	1.63	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	166	ARG	NE-CZ-NH2	-16.28	112.16	120.30
2	B	167	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	A	207	LEU	O-C-N	-12.12	103.31	122.70
2	B	167	ARG	NE-CZ-NH2	-9.09	115.76	120.30
2	B	177	ASP	CB-CG-OD2	9.01	126.41	118.30
2	B	166	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	113	ASP	CB-CG-OD2	8.32	125.79	118.30
2	B	169	ASP	CB-CG-OD2	7.28	124.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	328	ASP	CB-CG-OD2	7.27	124.84	118.30
2	B	170	ASP	CB-CG-OD2	7.21	124.79	118.30
2	B	338	ASP	CB-CG-OD2	7.03	124.62	118.30
1	A	179	ASP	CB-CG-OD2	6.63	124.27	118.30
2	B	249	MET	CG-SD-CE	-6.42	89.93	100.20
2	B	264	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	B	186	THR	OG1-CB-CG2	-5.94	96.33	110.00
2	B	245	ASP	CB-CG-OD2	5.74	123.46	118.30
2	B	229	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	319	ASP	CB-CG-OD2	5.63	123.36	118.30
2	B	196	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	166	ARG	NE-CZ-NH1	-5.09	117.75	120.30
2	B	347	LYS	N-CA-C	5.06	124.67	111.00
2	B	167	ARG	CG-CD-NE	-5.01	101.28	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	304	GLU	Peptide
2	B	305	LEU	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	1639	0	1653	12	0
2	B	1599	0	1584	31	0
3	A	115	0	0	4	1
3	B	61	0	0	5	0
All	All	3414	0	3237	41	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 6.

All (41) 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)
2:B:293:ASP:HB3	2:B:296:GLU:HG3	1.39	1.02
2:B:307:LYS:HE3	2:B:307:LYS:H	1.53	0.73
2:B:284:LYS:HE2	3:B:2053:HOH:O	1.91	0.71
2:B:316:MET:N	2:B:316:MET:SD	2.64	0.70
1:A:145:GLN:HE22	1:A:167:ILE:H	1.42	0.67
2:B:228:VAL:HG12	2:B:229:ASP:N	2.08	0.67
1:A:196:ARG:NH1	3:A:2109:HOH:O	2.27	0.65
1:A:162:GLU:HG2	3:A:2097:HOH:O	1.96	0.64
2:B:247:GLN:HE21	2:B:247:GLN:H	1.45	0.64
1:A:195:LYS:O	1:A:199:GLU:HG3	2.01	0.61
2:B:179:VAL:HG21	3:B:2040:HOH:O	2.03	0.59
2:B:228:VAL:CG1	2:B:229:ASP:N	2.69	0.56
2:B:179:VAL:HG12	2:B:231:ARG:HG2	1.90	0.54
2:B:316:MET:HE2	3:B:2057:HOH:O	2.08	0.52
2:B:181:LEU:O	2:B:186:THR:HG21	2.12	0.50
2:B:229:ASP:OD1	2:B:231:ARG:HB2	2.13	0.48
2:B:167:ARG:NH2	3:B:2017:HOH:O	2.46	0.48
2:B:200:GLU:O	2:B:201:GLU:HB2	2.14	0.48
2:B:329:ALA:O	2:B:333:MET:HB2	2.15	0.47
2:B:306:GLN:HB3	2:B:308:CYS:HB2	1.98	0.45
1:A:23:VAL:O	1:A:24:TYR:C	2.56	0.45
1:A:103:ALA:HB2	2:B:204:ALA:HB1	1.99	0.44
2:B:303:GLU:O	2:B:304:GLU:CB	2.66	0.44
1:A:78:ARG:NH2	3:A:2046:HOH:O	2.43	0.44
1:A:13:THR:HA	1:A:16:MET:HE2	2.00	0.44
2:B:185:GLU:HG3	3:B:2003:HOH:O	2.17	0.43
2:B:280:GLU:O	2:B:283:ARG:HB3	2.18	0.43
1:A:145:GLN:NE2	1:A:167:ILE:H	2.10	0.43
2:B:304:GLU:HB3	2:B:305:LEU:HD23	2.00	0.43
2:B:344:PRO:HB2	2:B:347:LYS:HA	2.01	0.43
1:A:183:GLU:HG3	1:A:189:ARG:HG2	2.01	0.43
2:B:158:GLN:HB3	2:B:181:LEU:HD11	2.00	0.42
1:A:109:SER:OG	2:B:202:LYS:NZ	2.52	0.42
2:B:319:ASP:O	2:B:322:SER:HB3	2.20	0.41
2:B:306:GLN:C	2:B:308:CYS:N	2.73	0.41
2:B:169:ASP:OD1	2:B:242:LYS:HE3	2.19	0.41
1:A:145:GLN:NE2	3:A:2085:HOH:O	2.54	0.41
2:B:181:LEU:O	2:B:186:THR:CG2	2.69	0.41
2:B:151:PHE:HE2	2:B:186:THR:HG22	1.85	0.41
2:B:196:ASP:O	2:B:200:GLU:HG3	2.21	0.40
2:B:228:VAL:CG1	2:B:229:ASP:H	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2007:HOH:O	3:A:2007:HOH:O[4_555]	2.03	0.17

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	205/214 (96%)	197 (96%)	8 (4%)	0	100	100
2	B	190/265 (72%)	177 (93%)	8 (4%)	5 (3%)	7	4
All	All	395/479 (82%)	374 (95%)	16 (4%)	5 (1%)	15	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	326	PRO
2	B	304	GLU
2	B	347	LYS
2	B	325	ASP
2	B	322	SER

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	181/189 (96%)	176 (97%)	5 (3%)	51	68
2	B	174/236 (74%)	154 (88%)	20 (12%)	7	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	355/425 (84%)	330 (93%)	25 (7%)	19	23

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	71	GLU
1	A	102	LYS
1	A	192	GLU
1	A	196	ARG
2	B	148	HIS
2	B	153	GLU
2	B	154	LYS
2	B	184	GLU
2	B	233	CYS
2	B	241	ILE
2	B	247	GLN
2	B	273	LYS
2	B	282	GLU
2	B	296	GLU
2	B	303	GLU
2	B	306	GLN
2	B	307	LYS
2	B	308	CYS
2	B	316	MET
2	B	321	ILE
2	B	323	LYS
2	B	324	MET
2	B	330	LYS
2	B	333	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	181	GLN
2	B	148	HIS
2	B	172	GLN
2	B	178	ASN
2	B	247	GLN

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

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, 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	207/214 (96%)	0.27	10 (4%) 34 43	15, 26, 51, 63	0
2	B	194/265 (73%)	0.77	29 (14%) 3 5	17, 38, 88, 101	0
All	All	401/479 (83%)	0.51	39 (9%) 10 14	15, 31, 76, 101	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	348	ALA	9.3
1	A	208	VAL	7.9
2	B	324	MET	6.4
2	B	321	ILE	5.9
2	B	346	SER	5.4
2	B	327	THR	4.7
2	B	308	CYS	4.2
2	B	148	HIS	4.2
2	B	232	ALA	4.2
2	B	323	LYS	4.2
1	A	114	VAL	3.8
2	B	345	ASN	3.8
2	B	149	LYS	3.7
2	B	326	PRO	3.3
1	A	200	PHE	3.2
2	B	347	LYS	3.2
2	B	325	ASP	3.0
2	B	319	ASP	2.9
2	B	328	ASP	2.8
2	B	318	GLN	2.7
1	A	207	LEU	2.6
2	B	303	GLU	2.6
2	B	330	LYS	2.5
2	B	329	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	227	LYS	2.4
1	A	117	ILE	2.4
2	B	280	GLU	2.3
1	A	50	LEU	2.3
2	B	333	MET	2.3
2	B	317	LEU	2.3
2	B	304	GLU	2.3
1	A	122	VAL	2.2
2	B	332	HIS	2.2
1	A	188	LYS	2.1
2	B	320	ALA	2.1
1	A	34	LEU	2.1
2	B	226	LEU	2.1
1	A	51	SER	2.1
2	B	240	LYS	2.0

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.