



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:36 pm GMT

PDB ID : 1QZE  
Title : HHR23a protein structure based on residual dipolar coupling data  
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Deposited on : 2003-09-16

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

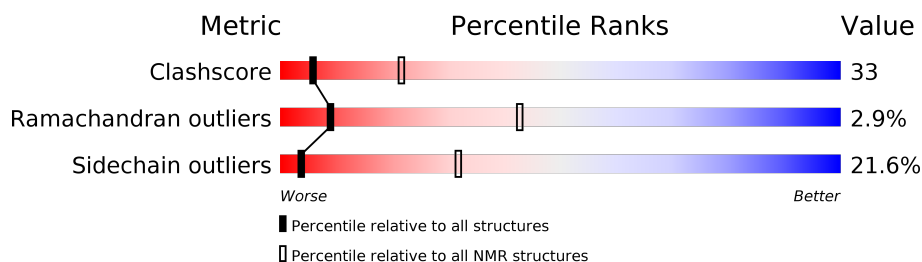
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	368	

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3490 atoms, of which 1756 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UV excision repair protein RAD23 homolog A.

Mol	Chain	Residues	Atoms						Trace
1	A	214	Total	C	H	N	O	S	0
			3490	1101	1756	298	327	8	

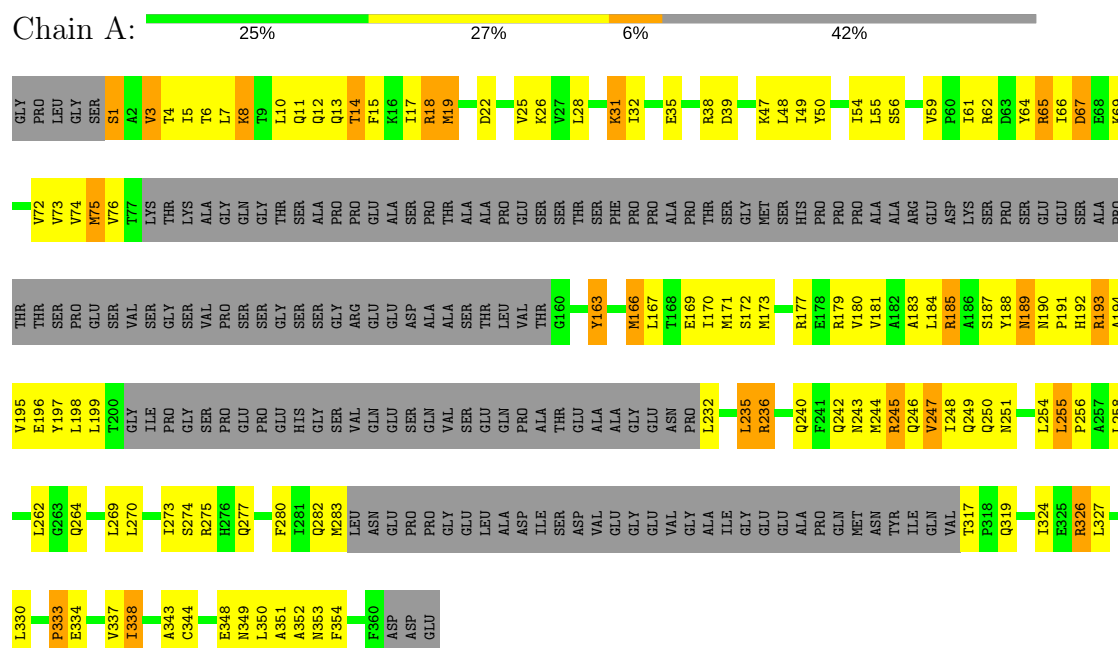
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P54725
A	-3	PRO	-	CLONING ARTIFACT	UNP P54725
A	-2	LEU	-	CLONING ARTIFACT	UNP P54725
A	-1	GLY	-	CLONING ARTIFACT	UNP P54725
A	0	SER	-	CLONING ARTIFACT	UNP P54725
A	1	SER	-	CLONING ARTIFACT	UNP P54725

## 4 Residue-property plots

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: UV excision repair protein RAD23 homolog A



## 5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
MODULE	structure solution	1.0
MODULE	refinement	1.0

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

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	Planarity
1	A	0	13
All	All	0	13

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	65	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	185	ARG	Sidechain
1	A	38	ARG	Sidechain
1	A	1	SER	Peptide
1	A	62	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	177	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	275	ARG	Sidechain
1	A	179	ARG	Sidechain
1	A	18	ARG	Sidechain

### 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1734	1756	1755	116
All	All	1734	1756	1755	116

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 33.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:49:ILE:CD1	1:A:54:ILE:HG22	0.90	1.97
1:A:334:GLU:O	1:A:338:ILE:HG22	0.82	1.74
1:A:49:ILE:HD13	1:A:54:ILE:HG22	0.71	1.61
1:A:25:VAL:HG23	1:A:59:VAL:O	0.71	1.86
1:A:49:ILE:HD11	1:A:54:ILE:HG22	0.71	1.63
1:A:343:ALA:HB2	1:A:351:ALA:HB2	0.68	1.66
1:A:8:LYS:O	1:A:74:VAL:HG12	0.66	1.91
1:A:180:VAL:O	1:A:184:LEU:HD13	0.65	1.91
1:A:327:LEU:HA	1:A:330:LEU:HD12	0.65	1.67
1:A:338:ILE:C	1:A:338:ILE:HD13	0.65	2.12
1:A:55:LEU:HD22	1:A:64:TYR:CG	0.62	2.29
1:A:163:TYR:CE1	1:A:181:VAL:CG2	0.62	2.83
1:A:170:ILE:HD13	1:A:184:LEU:HD11	0.61	1.72
1:A:349:ASN:O	1:A:353:ASN:N	0.61	2.34
1:A:7:LEU:HD11	1:A:48:LEU:CD1	0.59	2.27
1:A:269:LEU:HD23	1:A:273:ILE:HD12	0.58	1.74
1:A:25:VAL:HG11	1:A:56:SER:O	0.58	1.98
1:A:269:LEU:CD2	1:A:273:ILE:HD12	0.58	2.28
1:A:195:VAL:O	1:A:199:LEU:HD13	0.57	1.99
1:A:163:TYR:CE1	1:A:181:VAL:HG23	0.57	2.34
1:A:349:ASN:O	1:A:353:ASN:CB	0.57	2.53
1:A:28:LEU:HD13	1:A:61:ILE:HD13	0.56	1.77
1:A:163:TYR:C	1:A:163:TYR:CD1	0.56	2.78
1:A:343:ALA:HB2	1:A:351:ALA:CB	0.55	2.31
1:A:170:ILE:O	1:A:173:MET:HE2	0.55	2.01
1:A:55:LEU:HD22	1:A:64:TYR:CD1	0.55	2.37
1:A:188:TYR:CG	1:A:188:TYR:O	0.54	2.60
1:A:10:LEU:HD12	1:A:73:VAL:CG1	0.54	2.32
1:A:11:GLN:O	1:A:12:GLN:CB	0.53	2.56
1:A:7:LEU:CB	1:A:15:PHE:CE2	0.53	2.92
1:A:50:TYR:CB	1:A:55:LEU:HD11	0.53	2.34
1:A:197:TYR:CD1	1:A:197:TYR:N	0.52	2.73
1:A:32:ILE:HD13	1:A:74:VAL:HG21	0.52	1.80
1:A:183:ALA:O	1:A:187:SER:CB	0.52	2.58
1:A:187:SER:O	1:A:188:TYR:HB3	0.52	2.05

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:243:ASN:O	1:A:247:VAL:HG12	0.52	2.05
1:A:3:VAL:HG13	1:A:5:ILE:HD11	0.52	1.82
1:A:163:TYR:CE1	1:A:167:LEU:CD1	0.51	2.93
1:A:10:LEU:HD22	1:A:75:MET:HG2	0.51	1.82
1:A:194:ALA:O	1:A:198:LEU:N	0.51	2.44
1:A:349:ASN:O	1:A:350:LEU:C	0.51	2.49
1:A:167:LEU:HD23	1:A:180:VAL:CG1	0.50	2.36
1:A:343:ALA:CB	1:A:351:ALA:HB2	0.50	2.35
1:A:240:GLN:HB3	1:A:262:LEU:HD21	0.50	1.82
1:A:194:ALA:O	1:A:198:LEU:HG	0.50	2.06
1:A:269:LEU:HD21	1:A:280:PHE:CE2	0.49	2.42
1:A:47:LYS:HB3	1:A:54:ILE:CB	0.49	2.37
1:A:61:ILE:HD11	1:A:66:ILE:HD12	0.49	1.84
1:A:7:LEU:HB3	1:A:15:PHE:CE2	0.49	2.42
1:A:348:GLU:O	1:A:352:ALA:HB3	0.48	2.07
1:A:163:TYR:CE1	1:A:167:LEU:HD11	0.48	2.43
1:A:166:MET:CA	1:A:166:MET:HE3	0.48	2.39
1:A:255:LEU:N	1:A:256:PRO:HD2	0.48	2.23
1:A:235:LEU:HD12	1:A:269:LEU:HB2	0.48	1.83
1:A:166:MET:HA	1:A:169:GLU:HB2	0.47	1.86
1:A:324:ILE:HD12	1:A:338:ILE:HA	0.47	1.85
1:A:48:LEU:HD13	1:A:74:VAL:HB	0.47	1.85
1:A:166:MET:O	1:A:166:MET:CE	0.47	2.63
1:A:170:ILE:HG21	1:A:198:LEU:HD11	0.47	1.85
1:A:66:ILE:HG22	1:A:67:ASP:N	0.47	2.25
1:A:17:ILE:HG21	1:A:31:LYS:HG2	0.47	1.85
1:A:235:LEU:HD13	1:A:269:LEU:HD22	0.46	1.87
1:A:167:LEU:O	1:A:171:MET:CB	0.46	2.62
1:A:187:SER:HB2	1:A:193:ARG:C	0.46	2.30
1:A:15:PHE:CE2	1:A:35:GLU:HG2	0.46	2.46
1:A:183:ALA:O	1:A:187:SER:N	0.46	2.48
1:A:17:ILE:HG22	1:A:18:ARG:H	0.46	1.71
1:A:5:ILE:N	1:A:5:ILE:HD13	0.45	2.25
1:A:170:ILE:HD11	1:A:191:PRO:CA	0.45	2.41
1:A:18:ARG:O	1:A:19:MET:C	0.45	2.55
1:A:28:LEU:CD1	1:A:61:ILE:HD13	0.45	2.41
1:A:8:LYS:O	1:A:74:VAL:N	0.45	2.50
1:A:183:ALA:O	1:A:187:SER:HB3	0.45	2.12
1:A:180:VAL:HA	1:A:198:LEU:HD21	0.45	1.87
1:A:181:VAL:HA	1:A:184:LEU:HB2	0.45	1.89
1:A:167:LEU:HD23	1:A:180:VAL:HG12	0.44	1.88
1:A:327:LEU:CA	1:A:330:LEU:HD12	0.44	2.42

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:324:ILE:N	1:A:324:ILE:HD13	0.44	2.28
1:A:170:ILE:HD11	1:A:191:PRO:HA	0.44	1.89
1:A:190:ASN:O	1:A:194:ALA:CB	0.44	2.65
1:A:14:THR:C	1:A:15:PHE:CD1	0.44	2.90
1:A:49:ILE:HB	1:A:73:VAL:O	0.44	2.12
1:A:4:THR:C	1:A:5:ILE:HD13	0.44	2.33
1:A:193:ARG:O	1:A:197:TYR:N	0.43	2.48
1:A:3:VAL:HG13	1:A:3:VAL:O	0.43	2.14
1:A:18:ARG:O	1:A:19:MET:CG	0.43	2.66
1:A:333:PRO:O	1:A:337:VAL:HG21	0.43	2.14
1:A:50:TYR:CZ	1:A:66:ILE:HA	0.42	2.49
1:A:338:ILE:C	1:A:338:ILE:CD1	0.42	2.83
1:A:73:VAL:HG12	1:A:73:VAL:O	0.42	2.13
1:A:25:VAL:HG13	1:A:28:LEU:HD22	0.42	1.92
1:A:49:ILE:O	1:A:72:VAL:HG13	0.42	2.14
1:A:10:LEU:CD1	1:A:73:VAL:CG1	0.42	2.97
1:A:240:GLN:HA	1:A:262:LEU:HD11	0.42	1.90
1:A:163:TYR:CE1	1:A:167:LEU:HG	0.42	2.49
1:A:7:LEU:HD11	1:A:48:LEU:HD12	0.42	1.92
1:A:187:SER:HB2	1:A:193:ARG:CB	0.42	2.44
1:A:343:ALA:HB2	1:A:351:ALA:CA	0.42	2.45
1:A:188:TYR:O	1:A:189:ASN:C	0.42	2.58
1:A:194:ALA:O	1:A:197:TYR:N	0.42	2.53
1:A:273:ILE:CG2	1:A:274:SER:N	0.42	2.83
1:A:247:VAL:CG1	1:A:248:ILE:HD12	0.41	2.44
1:A:50:TYR:CD1	1:A:50:TYR:O	0.41	2.74
1:A:166:MET:CA	1:A:166:MET:CE	0.41	2.99
1:A:166:MET:O	1:A:166:MET:HE3	0.41	2.15
1:A:184:LEU:O	1:A:189:ASN:OD1	0.41	2.37
1:A:194:ALA:O	1:A:195:VAL:C	0.41	2.57
1:A:15:PHE:N	1:A:15:PHE:CD1	0.41	2.87
1:A:187:SER:HB2	1:A:194:ALA:N	0.41	2.30
1:A:243:ASN:O	1:A:247:VAL:CG1	0.41	2.68
1:A:258:LEU:CD1	1:A:258:LEU:N	0.41	2.83
1:A:350:LEU:CD2	1:A:350:LEU:N	0.41	2.84
1:A:255:LEU:HB3	1:A:256:PRO:HD3	0.41	1.93
1:A:170:ILE:O	1:A:171:MET:C	0.41	2.60
1:A:5:ILE:N	1:A:17:ILE:O	0.41	2.54
1:A:247:VAL:HG11	1:A:254:LEU:HD23	0.40	1.93

## 6.3 Torsion angles

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	206/368 (56%)	169 (82%)	31 (15%)	6 (3%)	9	43
All	All	206/368 (56%)	169 (82%)	31 (15%)	6 (3%)	9	43

All 6 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	3	VAL
1	A	76	VAL
1	A	19	MET
1	A	192	HIS
1	A	333	PRO
1	A	22	ASP

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	190/311 (61%)	149 (78%)	41 (22%)	4	32
All	All	190/311 (61%)	149 (78%)	41 (22%)	4	32

All 41 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	31	LYS
1	A	236	ARG
1	A	75	MET
1	A	247	VAL

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Mol	Chain	Res	Type
1	A	251	ASN
1	A	8	LYS
1	A	354	PHE
1	A	67	ASP
1	A	270	LEU
1	A	264	GLN
1	A	338	ILE
1	A	246	GLN
1	A	65	ARG
1	A	245	ARG
1	A	244	MET
1	A	166	MET
1	A	69	LYS
1	A	255	LEU
1	A	13	GLN
1	A	317	THR
1	A	14	THR
1	A	277	GLN
1	A	344	CYS
1	A	326	ARG
1	A	185	ARG
1	A	1	SER
1	A	250	GLN
1	A	283	MET
1	A	235	LEU
1	A	319	GLN
1	A	249	GLN
1	A	39	ASP
1	A	196	GLU
1	A	163	TYR
1	A	6	THR
1	A	282	GLN
1	A	172	SER
1	A	189	ASN
1	A	26	LYS
1	A	242	GLN
1	A	232	LEU

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided