

wwPDB NMR Structure Validation Summary Report (i)

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PDB ID : 1J4P

Title : NMR STRUCTURE OF THE FHA1 DOMAIN OF RAD53 IN COMPLEX

WITH A RAD9-DERIVED PHOSPHOTHREONINE (AT T155) PEPTIDE

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This is a wwPDB NMR 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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

ShiftChecker : 2.29

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	151	100%
2	В	13	100%



2 Ensemble composition and analysis (i)

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



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2644 atoms, of which 1333 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called PROTEIN KINASE SPK1.

Mol	Chain	Residues		Atoms									
1	Λ	151	Total	С	Н	N	О	S	0				
1	A	191	2424	751	1224	215	230	4	U				

• Molecule 2 is a protein called DNA REPAIR PROTEIN RAD9.

Mol	Chain	Residues		Atoms								
9	D	12	Total	С	Н	N	О	Р	S	0		
	Б	10	220	68	109	16	25	1	1	U		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	171	TPO	THR	modified residue	UNP P14737



4 Residue-property plots (i)

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: PROTEIN KINASE SPK1

Chain	A:															10	009	%																			
A14 T15 Q16 R17 F18	L19 I20 E21	K22 F23	\$24 025	E26	Q27 I28	G29	N31	132	C34	R35	V36 T37	C38 C38	T39	140 G41	Q42	I43 P44	145	R46	D47 L48	849	A50 D51	152	S53	U54 V55	1.56	K57	K59	R60	162	K63	K64	99M	T67	G69 G69	R70	P72	A73
C74 D75 Y76 H77 L78	G79 N80 I81	S82 R83	L84 S85	N86	K87 H88	F89	191	L92	G94	E95	D96 G97	86N	L99	L100	N102	D103 T104	\$105	T106	N107 G108	T109	W110	N112	G113	Q114 K115	V116	E117	N119	\$120	0122	L123	L124	Q126	G127	E129	I130	V132	G133
V134 G135 V136 E137 S138		S142 L143	V144 I145	F146	I147 N148			K152	Q153	L155	E156	N158	K159	V160 D161		I163																					
• Mole	ecule	e 2:	D	N.	A	Rl	ΕF	PΑ	ΙF	{]	PΕ	RC	Γ	Έ	IN	١]	R.	ΑI	Э9)																	
Chain	В:															10	00%	%																			
10 0 1 − 80 0	0 - 0	1 to 4	က်လ	7																																	



5 Refinement protocol and experimental data overview (i)



The models were refined using the following method: THE COMPLEX STRUCTURES ARE GENERATED USING A TOTAL OF 2438 RESTRAINTS. AMONG THEM, 3 ARTIFICAL CONSTRAINTS, 192 TALOS- DERIVED DIHEDRAL ANGLE RESTRAINS, 78 RESTRAINTS FROM H-BOND, 16 INTERMOLECULAR DISTANCE CONSTRAINS, AND 2149 INTRA-FHA1 AND INTRA- PEPTIDE DISTANCE CONSTRAINTS..

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
XwinNMR	structure solution	2.6
CNS	structure solution	1.0
CNS	refinement	1.0

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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	0	0	0	0
2	В	0	0	0	0
All	All	0	0	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 -.

There are no clashes.

6.3 Torsion angles (i)

6.3.1 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 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	0	-	-	-	-
2	В	0	-	-	-	-

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	0	-	=	-	-

There are no Ramachandran outliers.

6.3.2 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 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	0	-	-	-
2	В	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Pos	Link	Bo	nd lengt	ths
IVIOI	туре	Chain	rtes	Lilik	Bo Counts	RMSZ	#Z>2
2	TPO	В	171	2	8,10,11		0 (0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Trino	Chain	Dag	Timle	Bond angles				
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	#Z>2		
2	TPO	В	171	2	10,14,16	1.13	0 (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	TPO	В	171	2	-	0,9,11,13	-

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.

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

No chemical shift data were provided

