



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1Z00
Title : Solution structure of the C-terminal domain of ERCC1 complexed with the C-terminal domain of XPF
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Deposited on : 2005-03-01

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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 : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

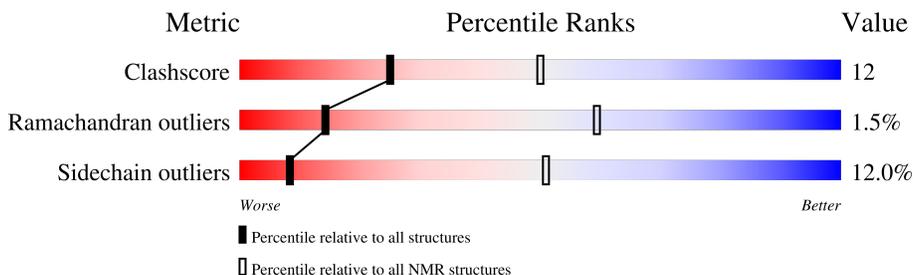
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	89	
2	B	84	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:231-A:295, B:833-B:894 (127)	0.15	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 9, 10, 12, 13, 15, 16, 17, 18, 19, 20
2	7, 8, 11, 14

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2614 atoms, of which 1318 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA excision repair protein ERCC-1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	84	1319	411	669	110	125	4	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	initiating methionine	UNP P07992
A	298	GLY	-	expression tag	UNP P07992
A	299	GLY	-	expression tag	UNP P07992
A	300	LEU	-	expression tag	UNP P07992
A	301	GLU	-	expression tag	UNP P07992
A	302	HIS	-	expression tag	UNP P07992
A	303	HIS	-	expression tag	UNP P07992
A	304	HIS	-	expression tag	UNP P07992
A	305	HIS	-	expression tag	UNP P07992
A	306	HIS	-	expression tag	UNP P07992
A	307	HIS	-	expression tag	UNP P07992

- Molecule 2 is a protein called DNA repair endonuclease XPF.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	84	1295	405	649	111	126	4	0

There is a discrepancy between the modelled and reference sequences:

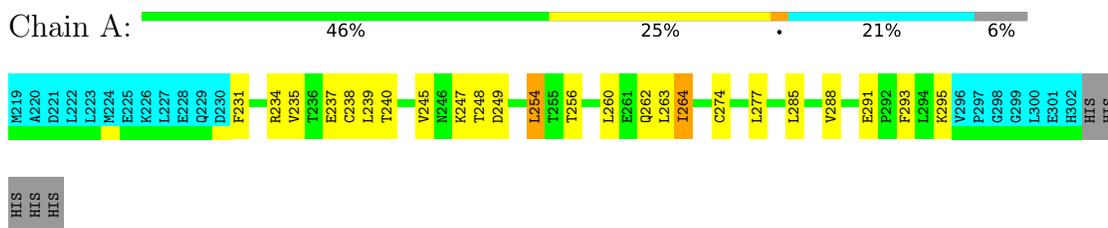
Chain	Residue	Modelled	Actual	Comment	Reference
B	822	MET	-	initiating methionine	UNP Q92889

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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: DNA excision repair protein ERCC-1



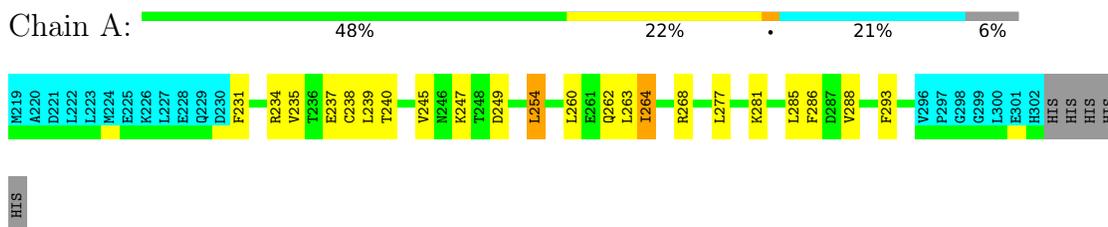
- Molecule 2: DNA repair endonuclease XPF



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 15. Colouring as in section 4.1 above.

- Molecule 1: DNA excision repair protein ERCC-1



- Molecule 2: DNA repair endonuclease XPF



M822	D623	S824	E825	T826	L827	P828	E829	S830	E831	K832	Y833	D839	F840	L841	L842	K843	M848	M851	C852	L855	Y859	K860	M861	T862	A863	E864	L868	S869	Q870	L873	L877	A883	L886	T892	S893	F894	A895	E896	V897	Y898	S899	K900	G901	K902	G903	K904	K905
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

5 Refinement protocol and experimental data overview

The models were refined using the following method: *water refinement in CNS*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	2.0
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	0.0±0.0	0.1±0.4
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	234	ARG	Sidechain	2
1	A	283	ARG	Sidechain	1

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	504	524	524	15±2
2	B	481	476	476	14±1
All	All	19700	20000	20000	461

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 12.

5 of 70 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:873:LEU:HD13	2:B:883:ALA:HB1	0.72	1.60	17	20
2:B:838:GLN:O	2:B:842:LEU:HG	0.70	1.87	7	2
1:A:235:VAL:O	1:A:239:LEU:HG	0.64	1.93	15	20
1:A:254:LEU:HD22	2:B:894:PHE:CZ	0.62	2.30	19	18
1:A:249:ASP:OD1	1:A:277:LEU:HD13	0.61	1.96	18	19

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	65/89 (73%)	60±1 (93±1%)	3±1 (5±2%)	1±1 (2±1%)	11	52
2	B	62/84 (74%)	60±1 (97±1%)	1±1 (2±1%)	1±0 (1±1%)	20	68
All	All	2540/3460 (73%)	2404 (95%)	97 (4%)	39 (2%)	14	59

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	295	LYS	16
2	B	845	PRO	13
1	A	276	GLY	9
1	A	275	PRO	1

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	58/79 (73%)	51±1 (88±2%)	7±1 (12±2%)	9	52
2	B	52/71 (73%)	46±1 (88±3%)	6±1 (12±3%)	8	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2200/3000 (73%)	1936 (88%)	264 (12%)	8 51

5 of 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	247	LYS	20
1	A	254	LEU	20
1	A	262	GLN	20
1	A	264	ILE	20
2	B	861	ASN	20

6.3.3 RNA [i](#)

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 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

No chemical shift data were provided