



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6FCV / pdb\_00006cv  
Title : Structure of the human DDB1-CSA complex  
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Deposited on : 2017-12-21  
Resolution : 2.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

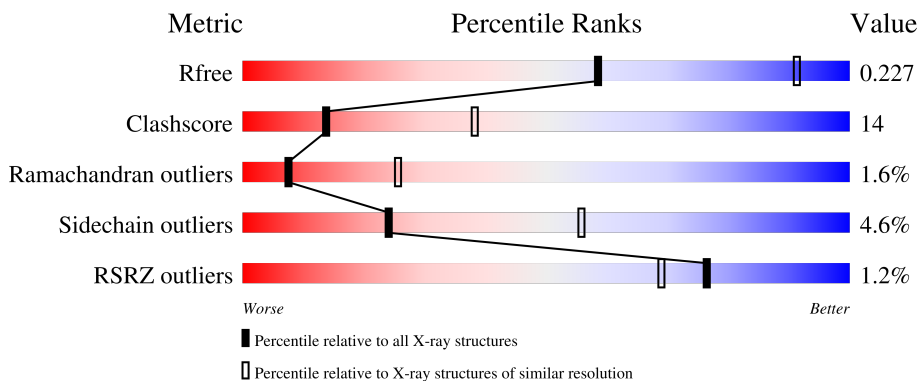
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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))
$R_{free}$	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	1158	 60% 32% • 6%
2	B	416	 57% 30% • 12%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11412 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1091	8563	5439	1443	1634	47	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	HIS	-	expression tag	UNP Q16531
A	-11	HIS	-	expression tag	UNP Q16531
A	-10	ARG	-	expression tag	UNP Q16531
A	-9	ARG	-	expression tag	UNP Q16531
A	-8	LEU	-	expression tag	UNP Q16531
A	-7	VAL	-	expression tag	UNP Q16531
A	-6	PRO	-	expression tag	UNP Q16531
A	-5	ARG	-	expression tag	UNP Q16531
A	-4	GLY	-	expression tag	UNP Q16531
A	-3	SER	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531

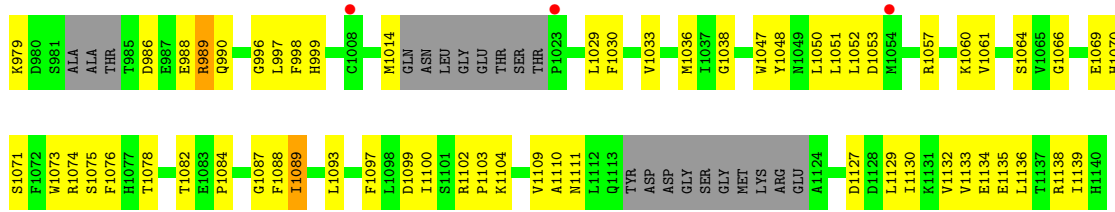
- Molecule 2 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	365	2849	1775	507	548	19	0	0	0

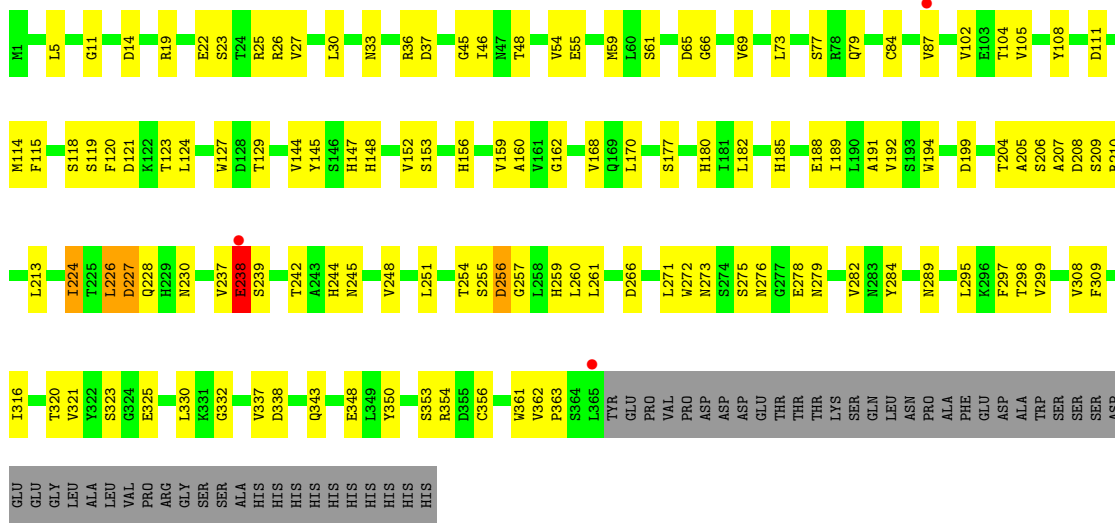
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	397	LEU	-	expression tag	UNP Q13216
B	398	ALA	-	expression tag	UNP Q13216
B	399	LEU	-	expression tag	UNP Q13216
B	400	VAL	-	expression tag	UNP Q13216
B	401	PRO	-	expression tag	UNP Q13216
B	402	ARG	-	expression tag	UNP Q13216
B	403	GLY	-	expression tag	UNP Q13216
B	404	SER	-	expression tag	UNP Q13216
B	405	SER	-	expression tag	UNP Q13216
B	406	ALA	-	expression tag	UNP Q13216
B	407	HIS	-	expression tag	UNP Q13216
B	408	HIS	-	expression tag	UNP Q13216
B	409	HIS	-	expression tag	UNP Q13216
B	410	HIS	-	expression tag	UNP Q13216
B	411	HIS	-	expression tag	UNP Q13216
B	412	HIS	-	expression tag	UNP Q13216
B	413	HIS	-	expression tag	UNP Q13216
B	414	HIS	-	expression tag	UNP Q13216
B	415	HIS	-	expression tag	UNP Q13216
B	416	HIS	-	expression tag	UNP Q13216





• Molecule 2: DNA excision repair protein ERCC-8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.79Å 140.79Å 249.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.67 – 2.92 68.67 – 2.92	Depositor EDS
% Data completeness (in resolution range)	88.7 (68.67-2.92) 90.1 (68.67-2.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.193 , 0.245 (Not available) , 0.227	Depositor DCC
$R_{free}$ test set	2923 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.9	Xtrriage
Anisotropy	0.004	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.81	3/8717 (0.0%)	0.75	5/11800 (0.0%)
2	B	0.95	2/2908 (0.1%)	0.75	2/3939 (0.1%)
All	All	0.85	5/11625 (0.0%)	0.75	7/15739 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLY	C-O	-6.58	1.18	1.24
2	B	226	LEU	C-O	-5.71	1.17	1.24
2	B	284	TYR	N-CA	5.31	1.53	1.46
1	A	999	HIS	CA-C	-5.21	1.46	1.52
1	A	139	LEU	C-O	5.08	1.29	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	THR	CA-C-N	5.59	126.83	119.84
1	A	544	THR	C-N-CA	5.59	126.83	119.84
2	B	14	ASP	CA-C-N	5.39	124.58	118.97
2	B	14	ASP	C-N-CA	5.39	124.58	118.97
1	A	837	TYR	CA-C-N	5.10	126.21	119.84

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	8563	0	8574	244	0
2	B	2849	0	2778	89	0
All	All	11412	0	11352	329	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 14.

The worst 5 of 329 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:30:LEU:HA	2:B:363:PRO:HA	1.42	1.01
2:B:152:VAL:HG11	2:B:199:ASP:HA	1.45	0.98
2:B:148:HIS:HD1	2:B:194:TRP:HD1	1.23	0.85
1:A:199:GLU:HG2	1:A:201:GLU:HB3	1.65	0.77
1:A:564:ILE:HG23	1:A:588:PRO:HD3	1.65	0.77

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	1075/1158 (93%)	941 (88%)	114 (11%)	20 (2%)	6	22
2	B	363/416 (87%)	326 (90%)	34 (9%)	3 (1%)	16	43
All	All	1438/1574 (91%)	1267 (88%)	148 (10%)	23 (2%)	7	25

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	ASP
1	A	1110	ALA
1	A	484	LYS

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Mol	Chain	Res	Type
1	A	544	THR
1	A	545	PRO

### 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	960/1014 (95%)	914 (95%)	46 (5%)	23 54
2	B	320/365 (88%)	307 (96%)	13 (4%)	27 60
All	All	1280/1379 (93%)	1221 (95%)	59 (5%)	24 56

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	676	VAL
2	B	260	LEU
1	A	849	VAL
2	B	256	ASP
2	B	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	852	GLN
2	B	9	GLN
2	B	326	GLN
1	A	1070	HIS
2	B	110	HIS

### 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 oligosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1091/1158 (94%)	0.10	14 (1%) 75 67	48, 92, 142, 175	0
2	B	365/416 (87%)	-0.17	3 (0%) 82 76	50, 74, 101, 145	0
All	All	1456/1574 (92%)	0.03	17 (1%) 76 69	48, 86, 138, 175	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	VAL	3.2
2	B	87	VAL	3.2
2	B	365	LEU	3.1
1	A	704	ILE	2.8
1	A	1008	CYS	2.7

### 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 oligosaccharides 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.