



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:05 pm GMT

PDB ID : 2B5M
Title : Crystal Structure of DDB1
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Deposited on : 2005-09-28
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

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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

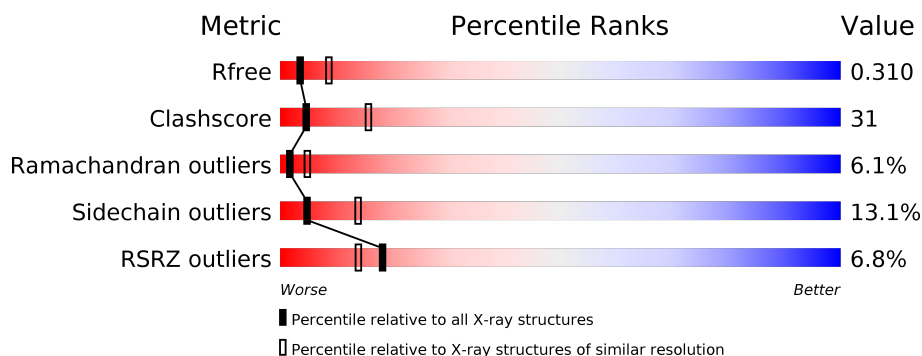
1 Overall quality at a glance

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}	100719	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (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 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	1140	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8768 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.

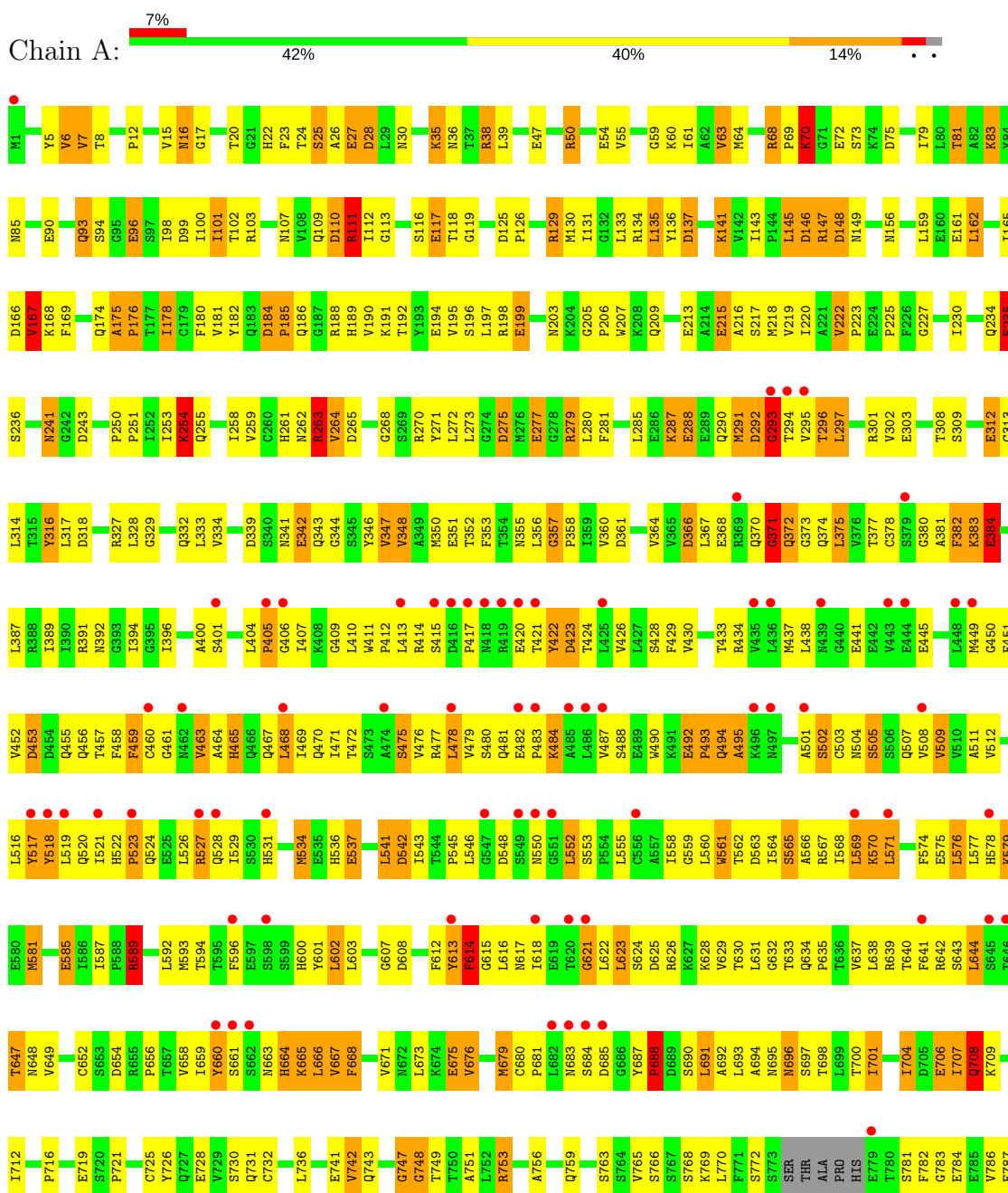
- Molecule 1 is a protein called damage-specific DNA binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1119	Total	C	N	O	S	0	0	0
			8768	5556	1477	1687	48			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: damage-specific DNA binding protein 1



V1108	V1109	A1110	N1111	L1112	G1N	T1R	ASP	GLY	GLY	SER	GLY	MET	LYS	R1122	E1123	A1124	T1125	D1128	L1129	I1130	K1131	V1132	V1133	E1134	E1135	L1136	T1137	R1138	I1139	H1140	Q1025	G1026	F1030	V1033	N1034	G1035	M1036	I1037	G1038	L1039	V1040	T1041	S1042	L1043	S1044	E1045	S1046	W1047	L1050	L1051	L1052	D1053	M1054	Q1055	L1058	N1059	V1065	G1066	E1069	W1073	E1079	R1080	P1084	A1085	T1086	I1089	D1090	G1091	D1092	L1093	I1094	E1095	S1096	F1097	I1100	S1101	R1102	P1103	K1104	R950	P951	N952	W953	N954	S955	A956	V957	E958	I959	L960	D961	D962	F965	L966	D969	R970	A971	F972	K979	D980	A983	T984	T985	D986	E987	F988	R989	Q990	H991	L992	Q993	F998	H999	L1000	G1001	E1002	F1003	V1004	F1007	L1012	V1013	M1014	Q1015	ASN	LEU	GLY	GLU	THR	SER	THR	P1023	T1024	N950	P951	N952	W953	N954	S955	A956	V957	E958	I959	L960	D961	D962	F965	L966	D969	R970	A971	F972	K979	D980	A983	T984	T985	D986	E987	F988	R989	Q990	H991	L992	Q993	F998	H999	L1000	G1001	E1002	F1003	V1004	F1007	L1012	V1013	M1014	Q1015	ASN	LEU	GLY	GLU	THR	SER	THR	P1023	T1024	L881	N885	S886	T887	V888	R889	W893	T894	T895	E896	K897	D898	V899	R900	T901	E902	C903	H904	H905	Y906	N907	N908	I909	M910	A911	L912	Y913	L914	K917	G918	D919	F920	V923	G924	D925	L926	N927	N928	S929	V930	L931	L932	K937	L933	M938	E939	G940	N941	E944	T945	A946	R947	D948	F949	V788	H789	I794	D795	Q796	H797	F798	F799	E800	H803	A804	H805	Q806	F807	L808	Y812	S815	L816	D824	P825	H826	T827	Y828	V831	E839	E840	A841	E842	P843	K844	T848	F851	Q852	Y853	S854	D855	Q856	K857	L858	T859	T860	V861	A862	E863	K864	E865	V866	S872	F876
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.38Å 133.83Å 184.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.92 48.68 – 2.92	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.70-2.92) 92.0 (48.68-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.277 0.293 , 0.310	Depositor DCC
R_{free} test set	1589 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8768	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, 0.333 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	1.62	110/8928 (1.2%)	1.41	85/12091 (0.7%)

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
1	A	1	2

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1033	VAL	CB-CG1	-10.01	1.31	1.52
1	A	277	GLU	CD-OE1	9.55	1.36	1.25
1	A	1135	GLU	CD-OE2	8.49	1.34	1.25
1	A	841	ALA	CA-CB	8.46	1.70	1.52
1	A	857	LYS	CD-CE	8.37	1.72	1.51

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	986	ASP	CB-CA-C	21.05	152.49	110.40
1	A	987	GLU	N-CA-CB	-18.34	77.60	110.60
1	A	842	GLU	N-CA-CB	-15.89	82.00	110.60
1	A	841	ALA	CB-CA-C	15.19	132.88	110.10
1	A	309	SER	N-CA-CB	-12.03	92.46	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	841	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1023	PRO	Peptide
1	A	292	ASP	Peptide

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	8768	0	8744	542	0
All	All	8768	0	8744	542	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 31.

The worst 5 of 542 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)
1:A:1054:MET:SD	1:A:1054:MET:CE	2.05	1.45
1:A:581:MET:SD	1:A:581:MET:CE	2.07	1.43
1:A:927:MET:CE	1:A:927:MET:SD	2.13	1.37
1:A:781:SER:HB3	1:A:784:GLU:OE1	1.31	1.27
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.07	1.09

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	1111/1140 (98%)	888 (80%)	155 (14%)	68 (6%)	2 5

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	A	291	MET
1	A	405	PRO
1	A	417	PRO
1	A	430	VAL

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	982/999 (98%)	853 (87%)	129 (13%)	5 14

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	TYR
1	A	602	LEU
1	A	1052	LEU
1	A	537	GLU
1	A	571	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	HIS
1	A	617	ASN
1	A	1055	GLN
1	A	455	GLN
1	A	456	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 [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, 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	1119/1140 (98%)	0.43	76 (6%) 18 14	8, 20, 29, 40	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	ASN	5.5
1	A	571	LEU	5.2
1	A	294	THR	4.9
1	A	508	VAL	4.9
1	A	660	TYR	4.6

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.