



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1MIU  
Title : Structure of a BRCA2-DSS1 complex  
Authors : Yang, H.; Jeffrey, P.D.; Miller, J.; Kinnucan, E.; Sun, Y.; Thoma, N.H.; Zheng, N.; Chen, P.L.; Lee, W.H.; Pavletich, N.P.  
Deposited on : 2002-08-23  
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

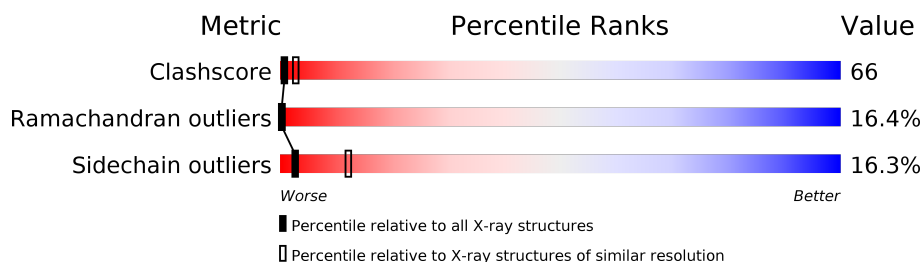
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	70	
2	A	738	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5647 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 Deleted in split hand/split foot protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	B	42	Total	C	N	O	0	0	0
			348	217	53	78			

- Molecule 2 is a protein called Breast Cancer type 2 susceptibility protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	671	Total	C	N	O	S	0	0	0
			5294	3361	925	991	17			

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

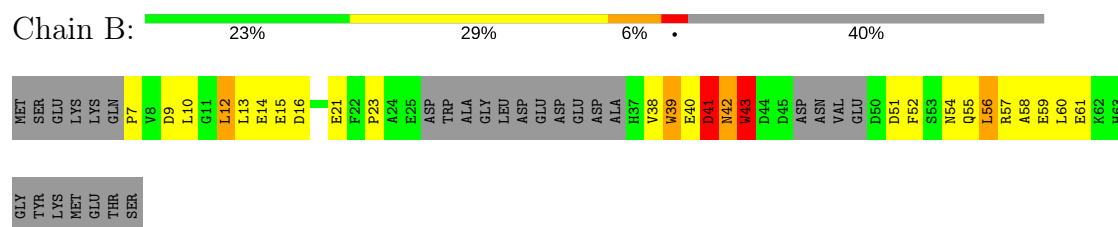
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Hg	0	0
			5	5		

### 3 Residue-property plots

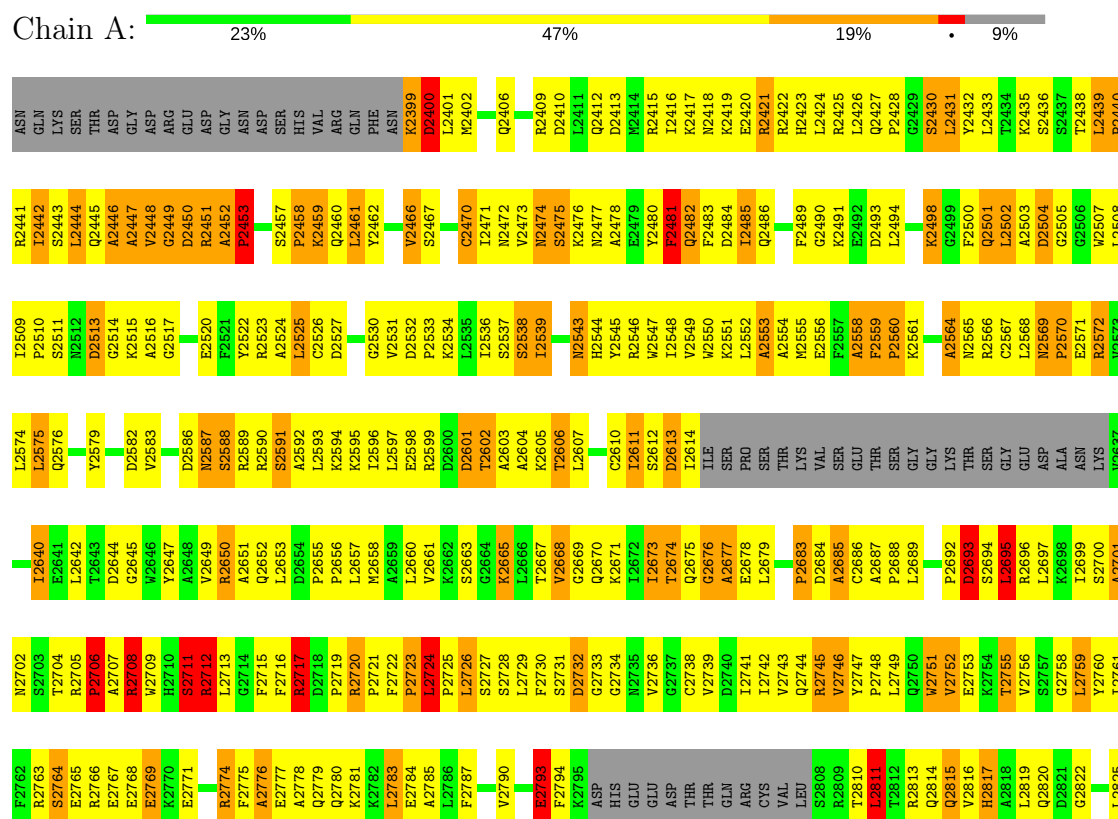
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

- Molecule 1: Deleted in split hand/split foot protein 1



- Molecule 2: Breast Cancer type 2 susceptibility protein



Y3091	Y2889	Y2854	V3021	V2889	V2829
K3092	W2890	V2854	V3024	K2891	Q2830
E3093	L2892	V2859	F3025	L2892	Y2831
A3094	L2893	S2960	G3026	S2961	A2832
E3095	V2894	S2966	D3027	V2895	S2833
K3096	T2895	L2865	L3028	S2896	D2834
K3097	D2896	Q2966	N3029	V2897	P2835
L3098	K2898	V2967	E3030	D2836	D2836
L3099	L2837	Y2968	D3031	K2899	H2837
	L2838	Q2969	I3032	K2899	L2838
L3102	E2839	P2970	K3033	K2900	E2839
E3103	A2840	R2971	P3034	E2901	E2840
GLY	C2841		R3035	K2902	C2841
ASP	F2842	L2974	V3036	S2903	F2842
SER	S2843	H2975	L3037	A2904	S2843
PRO	E2844	F2976	L3038	L2905	E2844
LYS	E2845	S2977	A3039	L2906	E2845
TRP	Q2846	R2978	A3040	S2907	Q2846
SER	L2847	L2979	S3041	I2908	L2847
THR	R2848	S2980	N3042	W2909	R2848
PRO	A2849	D2981	L3043	R2910	A2849
ASN	L2850	P2982	Q3044	P2911	L2850
LYS	N2851	A2983	C3045	S2912	N2851
ASP	N2852	F2984		S2913	N2852
	Y2853	Q2985	E3048	D2914	Y2853
	R2854	P2986	S3049	L2915	R2854
	Q2855	F2987	T3050		Q2855
	M2856	C2988	S3051	L2919	M2856
	L2857	S2989	G3052	T2920	L2857
	N2858	E2990	V3053	E2921	N2858
	D2859	V2991	P3054	G2922	D2859
	K2860	D2992	T3055	K2923	K2860
	K2861	V2993	L3056	R2924	K2861
	Q2862	V2994		Y2925	Q2862
	A2863	G2995	S3062	R2926	A2863
	R2864	V2996	I3063	I2927	R2864
	L2865	V2997		Y2928	L2865
	Q2866	V2998	P3068	H2929	Q2866
	S2867	S2999		L2930	S2867
	E2868	V3000	A3071	A2931	E2868
	F2869	V3001	Y3072	V2932	F2869
	K2870	K3002	F3073	S2933	K2870
	K2871	P3003	Q3074	K2934	K2871
	A2872	I3004	E3075	S2935	A2872
	L2873	G3005	K3076	R2936	L2873
	E2874	L3006	V3077	K2937	E2874
	S2875	A3007	N3078	F2938	S2875
	A2876	P3008	L3079	F2939	A2876
	E2877		L3080	E2940	E2877
	K2878		K3081	R2941	K2878
	E2880		H3082	P2942	E2880
	G2881		A3083	S2943	G2881
	L2882		I3084	D3014	L2882
	S2883		E3085	E3015	S2883
	R2884		N3086	C3016	R2884
			I3087	L3017	
			D3088	N3018	
			T3089	L3019	
			F3090	R2951	
				T2887	
				T2888	

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.51Å 228.27Å 81.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.256 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	B	0.57	0/354	0.85	2/478 (0.4%)
2	A	0.59	6/5399 (0.1%)	0.86	9/7303 (0.1%)
All	All	0.59	6/5753 (0.1%)	0.85	11/7781 (0.1%)

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
2	A	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2712	ARG	CZ-NH1	6.55	1.41	1.33
2	A	2712	ARG	CZ-NH2	6.13	1.41	1.33
2	A	2978	ARG	CZ-NH1	5.45	1.40	1.33
2	A	2978	ARG	CZ-NH2	5.41	1.40	1.33
2	A	3045	CYS	CB-SG	5.15	1.91	1.82

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2978	ARG	NE-CZ-NH1	11.80	126.20	120.30
2	A	2458	PRO	N-CA-CB	5.95	110.44	103.30
2	A	2811	LEU	CA-CB-CG	5.82	128.69	115.30
2	A	2724	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	7	PRO	N-CA-CB	5.45	109.83	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2853	TYR	Sidechain

## 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	B	348	0	281	59	0
2	A	5294	0	5280	722	0
3	A	5	0	0	0	0
All	All	5647	0	5561	744	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 66.

The worst 5 of 744 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:A:2936:LYS:HD3	2:A:2936:LYS:H	1.02	1.15
2:A:3001:VAL:HG12	2:A:3003:PRO:HD3	1.34	1.05
2:A:2426:LEU:H	2:A:2426:LEU:HD12	1.20	1.01
1:B:9:ASP:HB3	1:B:12:LEU:HD12	1.42	0.99
2:A:3020:LEU:HA	2:A:3054:PRO:HD2	1.47	0.97

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	B	36/70 (51%)	25 (69%)	7 (19%)	4 (11%)	0	2
2	A	665/738 (90%)	427 (64%)	127 (19%)	111 (17%)	0	0
All	All	701/808 (87%)	452 (64%)	134 (19%)	115 (16%)	0	0

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ASP
1	B	56	LEU
2	A	2440	PRO
2	A	2451	ARG
2	A	2453	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	B	36/63 (57%)	32 (89%)	4 (11%)	7	29
2	A	571/649 (88%)	476 (83%)	95 (17%)	2	11
All	All	607/712 (85%)	508 (84%)	99 (16%)	3	12

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2746	VAL
2	A	2841	CYS
2	A	3041	SER
2	A	2752	VAL
2	A	2783	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2814	GLN
2	A	2855	GLN
2	A	3044	GLN
2	A	2670	GLN
2	A	2675	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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

### 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.