



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 09:08 am BST

PDB ID : 1IYJ  
Title : STRUCTURE OF A BRCA2-DSS1 COMPLEX  
Authors : Pavletich, N.P.; Jeffrey, P.D.; Yang, H.J.  
Deposited on : 2002-08-28  
Resolution : 3.40 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.

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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  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

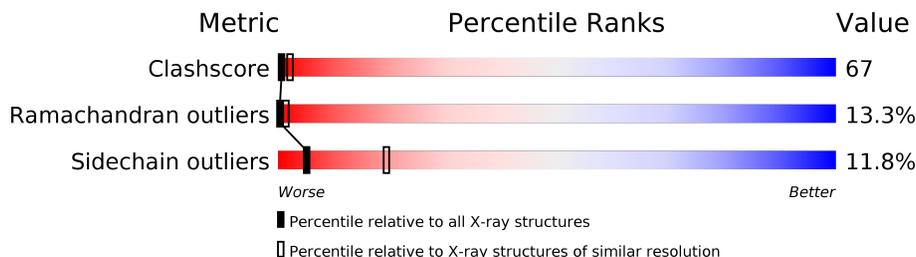
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	70	 10% 33% 21% 36%
1	C	70	 7% 33% 24% 36%
2	B	817	 15% 45% 12% • 28%
2	D	817	 17% 43% 12% • 28%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10092 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
			Total	C	N	O			
1	A	45	380	235	59	86	0	0	0
1	C	45	380	235	59	86	0	0	0

- Molecule 2 is a protein called breast cancer susceptibility.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	591	4666	2984	805	862	15	0	0	0
2	D	591	4666	2984	805	862	15	0	0	0

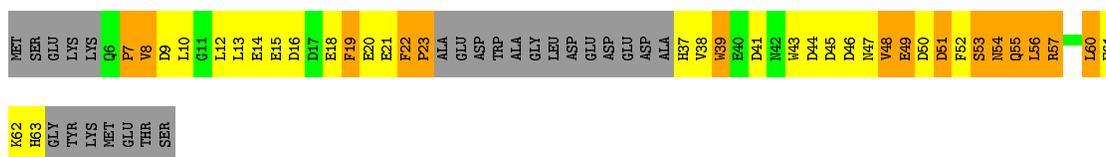
### 3 Residue-property plots [i](#)

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. 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. 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.

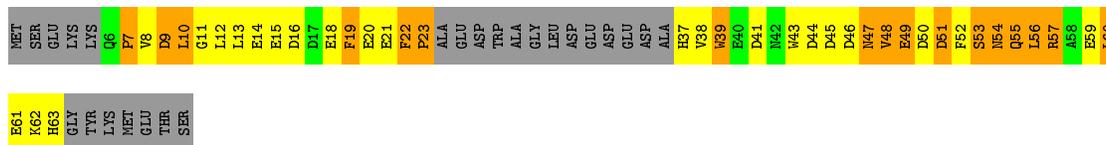
- Molecule 1: Deleted in split hand/split foot protein 1

Chain A: 



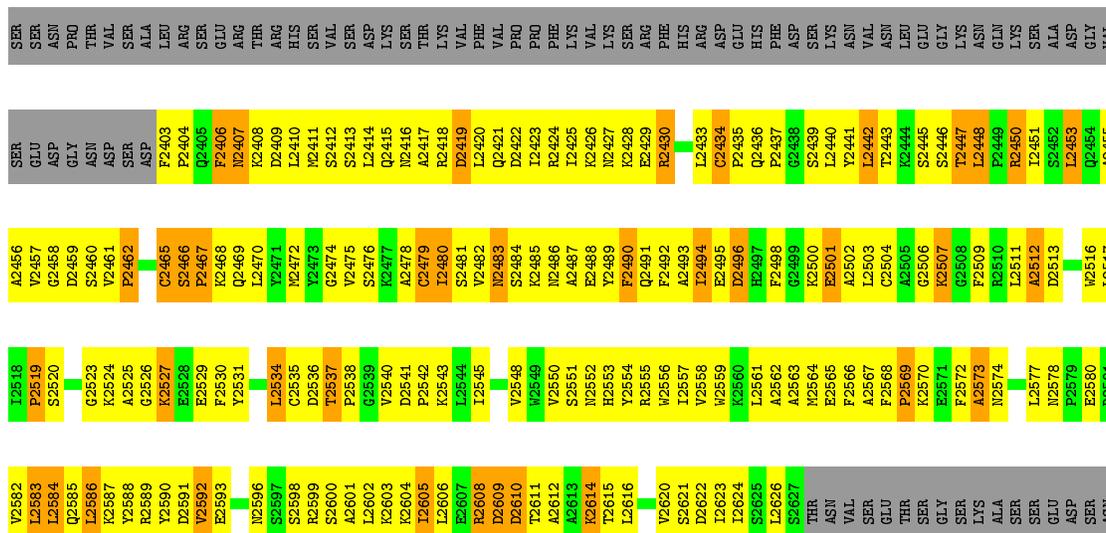
- Molecule 1: Deleted in split hand/split foot protein 1

Chain C: 



- Molecule 2: breast cancer susceptibility

Chain B: 



T2652	D2652	K2652	L2652	M2652	N2652	P2652	Q2652	R2652	S2652	T2652	V2652	W2652	X2652	Y2652	Z2652
D2653	L2653	K2653	L2653	M2653	N2653	P2653	Q2653	R2653	S2653	T2653	V2653	W2653	X2653	Y2653	Z2653
D2654	L2654	K2654	L2654	M2654	N2654	P2654	Q2654	R2654	S2654	T2654	V2654	W2654	X2654	Y2654	Z2654
D2655	L2655	K2655	L2655	M2655	N2655	P2655	Q2655	R2655	S2655	T2655	V2655	W2655	X2655	Y2655	Z2655
D2656	L2656	K2656	L2656	M2656	N2656	P2656	Q2656	R2656	S2656	T2656	V2656	W2656	X2656	Y2656	Z2656
D2657	L2657	K2657	L2657	M2657	N2657	P2657	Q2657	R2657	S2657	T2657	V2657	W2657	X2657	Y2657	Z2657
D2658	L2658	K2658	L2658	M2658	N2658	P2658	Q2658	R2658	S2658	T2658	V2658	W2658	X2658	Y2658	Z2658
D2659	L2659	K2659	L2659	M2659	N2659	P2659	Q2659	R2659	S2659	T2659	V2659	W2659	X2659	Y2659	Z2659
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D2673	L2673	K2673	L2673	M2673	N2673	P2673	Q2673	R2673	S2673	T2673	V2673	W2673	X2673	Y2673	Z2673
D2674	L2674	K2674	L2674	M2674	N2674	P2674	Q2674	R2674	S2674	T2674	V2674	W2674	X2674	Y2674	Z2674
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D2677	L2677	K2677	L2677	M2677	N2677	P2677	Q2677	R2677	S2677	T2677	V2677	W2677	X2677	Y2677	Z2677
D2678	L2678	K2678	L2678	M2678	N2678	P2678	Q2678	R2678	S2678	T2678	V2678	W2678	X2678	Y2678	Z2678
D2679	L2679	K2679	L2679	M2679	N2679	P2679	Q2679	R2679	S2679	T2679	V2679	W2679	X2679	Y2679	Z2679
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D2681	L2681	K2681	L2681	M2681	N2681	P2681	Q2681	R2681	S2681	T2681	V2681	W2681	X2681	Y2681	Z2681
D2682	L2682	K2682	L2682	M2682	N2682	P2682	Q2682	R2682	S2682	T2682	V2682	W2682	X2682	Y2682	Z2682
D2683	L2683	K2683	L2683	M2683	N2683	P2683	Q2683	R2683	S2683	T2683	V2683	W2683	X2683	Y2683	Z2683
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D2701	L2701	K2701	L2701	M2701	N2701	P2701	Q2701	R2701	S2701	T2701	V2701	W2701	X2701	Y2701	Z2701
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D2703	L2703	K2703	L2703	M2703	N2703	P2703	Q2703	R2703	S2703	T2703	V2703	W2703	X2703	Y2703	Z2703
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D2732	L2732	K2732	L2732	M2732	N2732	P2732	Q2732</								

E3094	K2716	GLN	ASP	W2899	R2960	C3025	E3094
M3095	K2717	ASP	ASP	K2900	T2961	L3026	M3095
I3096	A2781	ALA	ALA	L2901	L2966	H3027	I3096
D3097	L2782	SER	SER	R2902	L2967	L3028	D3097
F3099	S2720	ASP	ASP	V2903	V2968	I3029	F3099
V3100	K2721	PRO	PRO	T2904	S2969	V3030	V3100
K3101	ALA	ALA	ALA	S2905	S2970	V3031	K3101
E3102	GLU	GLU	GLU	Y2906	E2971	K3032	E3102
A3103	F2724	ALA	ALA	K2907	E2972	G3034	A3103
E3104	F2725	ALA	ALA	K2908	L2972	I3035	E3104
K3105	H2726	GLN	GLN	R2909	L2973	D3036	K3105
K3106	R2729	CYS	CYS	E2910	L2974	L3037	K3106
L3107	R2730	LYS	LYS	K2911	Q2975	M3038	L3107
Q3108	F2731	SER	SER	S2912	Q2978	E3039	Q3108
Q3109	P2732	GLU	GLU	A2913	P2979	D3040	Q3109
V3110	L2733	ALA	ALA	L2914	R2980	I3041	V3110
L3111	P2734	GLN	GLN	L2915	E2981	K3042	L3111
L3112	L2735	LEU	LEU	S2916	L2982	P3043	L3112
G3113	S2736	THR	THR	W2917	L2983	R3044	G3113
D3114	S2737	LYS	LYS	M2918	P2984	V3045	D3114
S3115	F2739	HIS	HIS	R2919	F2985	L3046	S3115
P3116	S2740	THR	THR	S2920	K2987	I3047	P3116
K3117	D2741	TYR	TYR	S2922	L2988	A3048	K3117
THR	G2742	LEU	LEU	D2923	S2989	A3049	THR
SER	G2743	ARG	ARG	L2924	D2990	S3050	SER
THR	N2744	GLN	GLN	P2925	P2991	N3051	THR
PRO	V2745	MET	MET	S2926	A2992	W3054	PRO
ASN	G2746	LEU	LEU	L2927	F2993	R3055	ASN
LYS	C2747	SER	SER	L2928	F2994	P3056	LYS
ASP	V2748	ASP	ASP	T2929	Q2994	E3057	ASP
PRO	S2749	LYS	LYS	E2930	P2995	S3058	PRO
THR	L2750	LYS	LYS	G2931	P2996	L3064	THR
ARG	L2751	ALA	ALA	R2932	C2997	T3064	ARG
GLU	V2752	ALA	ALA	R2933	E2998	L3065	GLU
PRO	Q2753	ARG	ARG	Y2934	E2999	F3066	PRO
TYR	R2754	ARG	ARG	R2935	V3000	G3068	TYR
PRO	V2755	VAL	VAL	L2936	D3001	F3070	PRO
ALA	K2756	LEU	LEU	Y2937	V3002	S3071	ALA
SER	P2757	SER	SER	H2938	V3005	H3081	SER
THR	L2758	ARG	ARG	L2939	V3006	F3082	THR
CYS	Q2759	ALA	ALA	S2940	V3007	Q3083	CYS
SER	W2760	THR	THR	S2942	S3008	E3084	SER
ALA	V2761	ALA	ALA	K2943	V3009	R3085	ALA
SER	E2762	GLN	GLN	S2944	V3010	V3086	SER
ASP	T2764	VAL	VAL	R2945	K3011	T3087	ASP
LEU	V2765	ALA	ALA	N2946	L3012	M3088	LEU
SER	S2766	GLU	GLU	E2949	L3013	K3089	SER
GLY	G2767	LEU	LEU	M2950	G3014	K3090	GLY
GLY	S2768	GLN	GLN	P2951	L3015	H3091	GLY
GLN	Y2769	ASP	ASP	S2952	A3016	A3092	GLN
GLY	R2772	GLY	GLY	T2953	P3017	D3023	GLY
ALA	N2773	ALA	ALA	Q2954	L3018	I3093	ALA
LEU	F2774	LEU	LEU	L2955	V3019		LEU
THR	K2775	THR	THR	T2956	L3021		THR
ALA	E2776	ALA	ALA	A2957	S3022		ALA
E2777	A2777	ALA	ALA	T2958	D3023		E2777
E2778	VAL	VAL	VAL	K2959	E3024		E2778

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.31Å 130.31Å 192.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.244 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 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	0.42	0/388	0.80	1/526 (0.2%)
1	C	0.41	0/388	0.80	1/526 (0.2%)
2	B	0.42	0/4774	0.71	2/6475 (0.0%)
2	D	0.42	0/4774	0.71	3/6475 (0.0%)
All	All	0.42	0/10324	0.71	7/14002 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2467	PRO	N-CA-CB	6.04	110.54	103.30
2	D	2467	PRO	N-CA-CB	5.96	110.45	103.30
1	A	7	PRO	N-CA-CB	5.61	110.03	103.30
1	C	7	PRO	N-CA-CB	5.50	109.90	103.30
2	D	2941	VAL	N-CA-C	-5.50	96.16	111.00

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	380	0	306	61	0
1	C	380	0	306	66	0
2	B	4666	0	4694	652	0
2	D	4666	0	4694	629	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10092	0	10000	1356	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 67.

The worst 5 of 1356 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:D:2683:THR:HG22	2:D:2713:THR:HB	1.22	1.16
2:D:2750:VAL:HG11	2:D:2903:VAL:HB	1.18	1.16
2:B:2683:THR:HG22	2:B:2713:THR:HB	1.20	1.13
2:B:2750:VAL:HG11	2:B:2903:VAL:HB	1.19	1.12
2:B:2942:SER:HB3	2:B:2953:ILE:HD11	1.39	1.03

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	41/70 (59%)	18 (44%)	11 (27%)	12 (29%)	0	0
1	C	41/70 (59%)	18 (44%)	11 (27%)	12 (29%)	0	0
2	B	585/817 (72%)	387 (66%)	128 (22%)	70 (12%)	0	3
2	D	585/817 (72%)	391 (67%)	122 (21%)	72 (12%)	0	2
All	All	1252/1774 (71%)	814 (65%)	272 (22%)	166 (13%)	0	1

5 of 166 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	47	ASN

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Mol	Chain	Res	Type
1	A	51	ASP
1	A	53	SER
1	A	57	ARG

### 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	41/63 (65%)	33 (80%)	8 (20%)	1 4
1	C	41/63 (65%)	33 (80%)	8 (20%)	1 4
2	B	517/721 (72%)	459 (89%)	58 (11%)	6 22
2	D	517/721 (72%)	459 (89%)	58 (11%)	6 22
All	All	1116/1568 (71%)	984 (88%)	132 (12%)	5 19

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3062	VAL
1	C	60	LEU
2	D	3040	ASP
2	B	3081	HIS
1	C	19	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3095	ASN
2	D	2436	GLN
2	D	3083	GLN
1	C	54	ASN
2	B	2596	ASN

### 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

### 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.