



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1MIU / pdb_00001miu
Title : Structure of a BRCA2-DSS1 complex
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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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

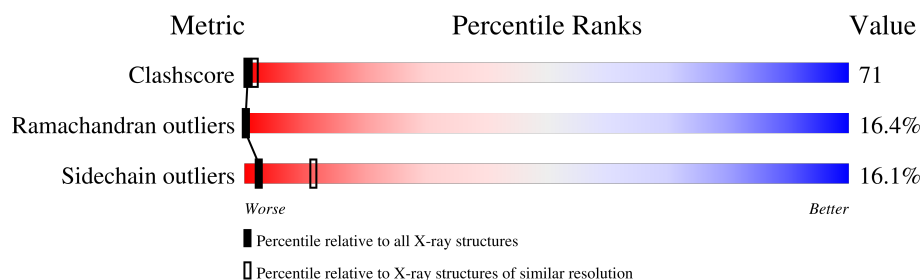
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 ≥ 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	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 (CCD ID: HG) (formula: Hg).

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

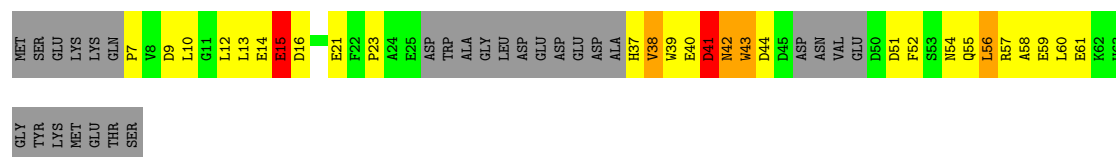
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

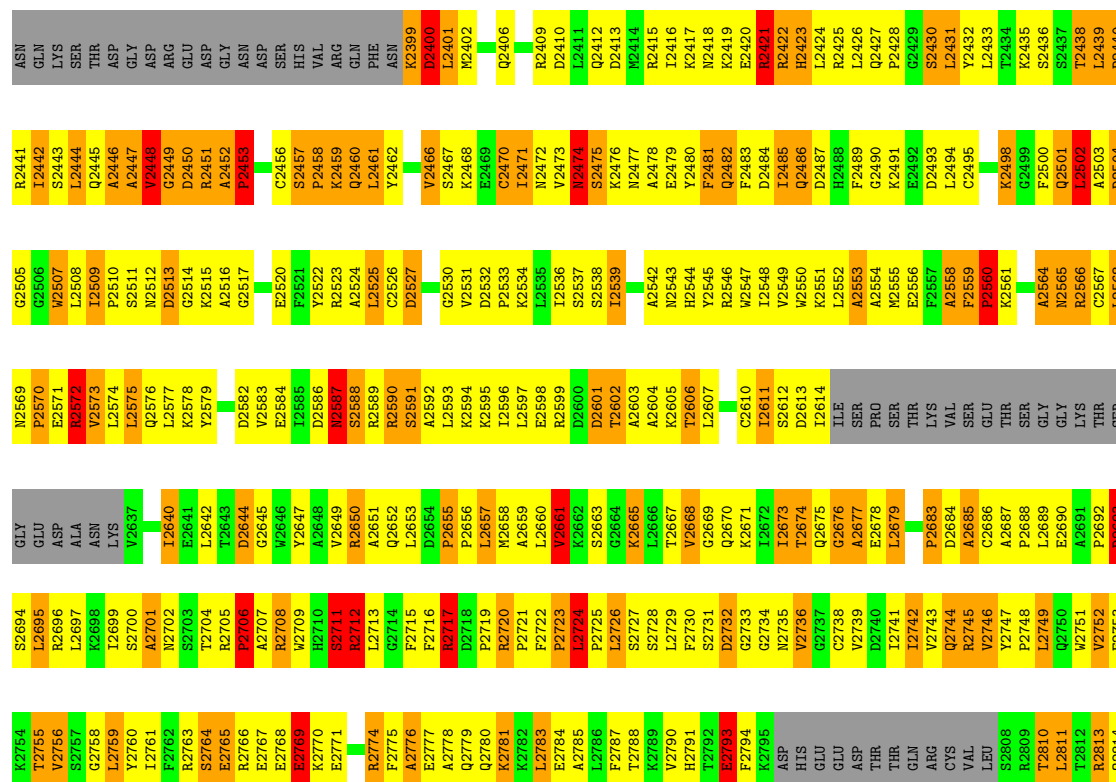
- Molecule 1: Deleted in split hand/split foot protein 1

Chain B: 



- Molecule 2: Breast Cancer type 2 susceptibility protein

Chain A: 



L3080	K3081	H3082	A3083	L3084	E3085	N3086	I3087	D3088	T3089	F3090	Y3091	K3092	E3093	A3094	E3095	K3096	K3097	L3098	I3099	L3102	E3103	GLY	ASP	SER	PRO	LYS	TRP	SER	THR	PRO	ASN	LYS	ASP																															
G3005	L3006	A3007	F3008	Y3011	L3012	S3013	D3014	E3015	C3016	L3017		L3018	L3019	L3020	V3021	F3024	G3025	I3026	D3027	L3028	N3029	E3030	D3031	I3032	K3033	F3034	R3035	V3036	L3037	I3038	A3039	S3041	N3042	L3043	T3050	S3051	G3052	V3053	P3054	T3055	L3056	S3062	I3063	P3068	A3071	Y3072	F3073	Q3074	E3075	K3076	V3077	N3078	N3079											
S2937	K2938	F2939	E2940	R2941	P2942	S2943	I2944	Q2945	L2946	T2947		R2951	T2952	Q2953	Y2954	V2959	S2960	S2961	L2965	Q2966	V2967	Y2968	Q2969	P2970	R2971	L2974	H2975	F2976	S2977	R2978	L2979	S2980	D2981	P2982	A2983	F2984	Q2985	P2986	P2987	C2988	S2989	E2990	V2991	D2992	V2993	V2994	G2995	V2996	V2997	V2998	S2999	V3000	V3001	V3002	K3003	P3003	L3004							
S2875	V2876	E2877	K2878	E2879	E2880	G2881	L2882	S2883	R2884	D2885	V2886	T2887	T2888	V2889	K2891	L2892	R2893	V2894	T2895	S2896	Y2897	K2898	K2899	K2900	E2901	K2902	F2842	S2843	A2904	E2845	L2906	S2907	L2847	R2848	A2849	R2910	L2850	N2851	N2852	Y2853	R2854	Q2855	L2915		L2919	T2920	N2858	E2921	R2859	K2860	K2861	Q2862	A2863	R2864	L2865	Q2866	S2867	E2868	F2869	R2870	V2871	A2872	L2873	K2936

4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	Xtriage
Total number of atoms	5647	wwPDB-VP
Average B, all atoms (Å ²)	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	0.66	0/354	1.16	3/478 (0.6%)
2	A	0.74	6/5399 (0.1%)	1.29	78/7303 (1.1%)
All	All	0.74	6/5753 (0.1%)	1.28	81/7781 (1.0%)

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	6.30	1.41	1.32
2	A	2472	ASN	CG-OD1	6.15	1.35	1.23
2	A	2712	ARG	CZ-NH2	5.82	1.41	1.33
2	A	2978	ARG	NE-CZ	5.66	1.39	1.33
2	A	2978	ARG	CZ-NH1	5.27	1.40	1.32

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2844	GLU	N-CA-C	11.50	118.21	108.78
2	A	2422	ARG	N-CA-C	10.70	122.83	108.07
2	A	2724	LEU	CA-C-N	8.88	129.58	119.99
2	A	2724	LEU	C-N-CA	8.88	129.58	119.99
2	A	2769	GLU	N-CA-C	-8.83	103.34	114.56

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	61	0
2	A	5294	0	5280	767	0
3	A	5	0	0	0	0
All	All	5647	0	5561	791	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 71.

The worst 5 of 791 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:H	2:A:2936:LYS:HD3	1.02	1.15
2:A:3001:VAL:HG12	2:A:3003:PRO:HD3	1.34	1.05
2:A:2426:LEU:HD12	2:A:2426:LEU:H	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%)	33 (92%)	3 (8%)	10	35
2	A	571/649 (88%)	476 (83%)	95 (17%)	2	10
All	All	607/712 (85%)	509 (84%)	98 (16%)	2	11

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2856	MET
2	A	2915	LEU
2	A	2864	ARG
2	A	2892	LEU
2	A	2936	LYS

Sometimes 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	2956	GLN
2	A	3078	ASN
2	A	3086	ASN
2	A	3079	ASN
2	A	2587	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 oligosaccharides 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.