



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:23 PM UTC

PDB ID : 1MJE / pdb_00001mje
Title : STRUCTURE OF A BRCA2-DSS1-SSDNA COMPLEX
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Deposited on : 2002-08-27
Resolution : 3.50 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

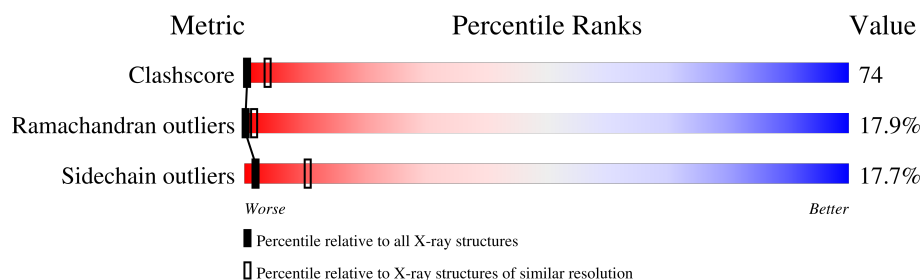
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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	C	6	100%
2	B	70	14% 26% 17% . 40%
3	A	649	17% 45% 25% 5% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5198 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 DNA chain called 5'-D(P*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	6	Total	C	N	O	P	16	0	0
			121	60	12	43	6			

- Molecule 2 is a protein called Deleted in split hand/split foot protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	42	Total	C	N	O	0	0	0
			335	209	50	76			

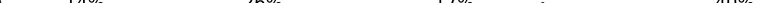
- Molecule 3 is a protein called breast cancer 2.

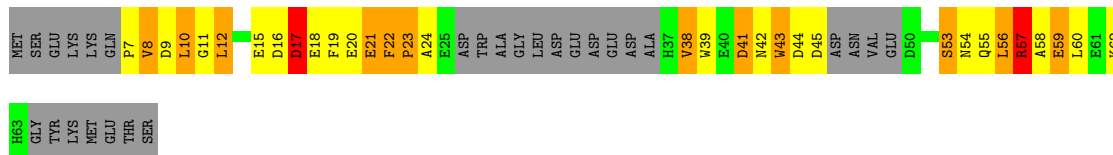
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	600	Total	C	N	O	S	0	0	0
			4742	3025	824	877	16			

Note EDS was not executed.

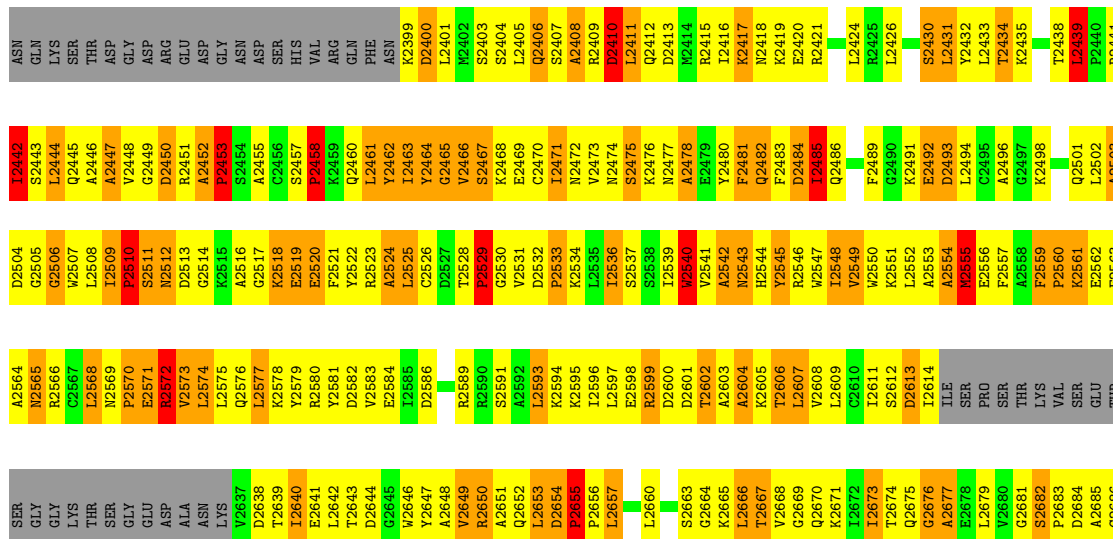
- Chain C: 100%



- Chain B: 



- Chain A: 17% 45% 25% 5% 8%



Y3092	K3093	E3094	A3095	E3096	K3097	K3098	L3099	I3100	H3101	V3102	L3103		D3106	S3107	P3108	K3109	W3110	SER	THR	PRO	ASN																																								
L3028	N3029	E3030	D3031	I3032	K3033	P3034	R3035	V3036	L3037	I3038	A3039	A3040	S3041	N3042	L3043	Q3044	G3045	Q3046	P3047	E3048	S3049	T3050	S3051	G3052	V3053	P3054	L3056	F3057	A3058	C3059	H3060	S3061	I3062	I3063		S3067		E3070	A3071	V3072	F3073	Q3074	E3075	K3076	V3077	N3078	N3079	L3080	K3081	H3082	A3083	I3084	E3085	N3086	I3087	D3089	T3090	F3091			
E2962	T2963	L2964	L2965	Q2966	V2967	Y2968	Q2969	P2970	R2971		L2974	H2975	F2976	S2977	R2978	L2979	S2980	D2981	P2982	A2983	F2984	Q2985	P2986	C2987	C2988	S2989	E2990	V2991	D2992	H2993	V2994		V2997	V2998	S2999	V3000	V3001	A3002	P3003	I3004	G3005	L3006	A3007	P3008	L3009	V3010	Y3011	L3012	S3013	D3014		L3017	N3018	L3019	L3020	V3021		F3024			
S2896	Y2897	K2898	K2899	K2900	E2901	K2902	A2903	L2904	L2905	L2906	S2907	T2908	W2909	R2910	P2911	S2912	S2913	D2914	L2915		L2919		G2922	K2923	R2924	Y2925	R2926	L2927	Y2928	H2929	L2930	A2931	V2932	S2933	K2934	S2935	K2936	S2937	K2938	F2939	E2940	R2941	P2942		Q2945	L2946	T2947		R2951	T2952	Q2953	Y2954	Q2955	Q2956	L2957	P2958	V2959	S2960	S2961		
P2748	L2749	Q2750	W2751	V2752	E2753	K2754	T2755	V2756	S2757	G2758	L2759	Y2760	I2761	F2762	K2763	S2764	E2765	R2766	E2767	E2768	R2769	K2770	E2771	A2772	L2773	R2774	F2775	A2776		Q2779	Q2780	K2781	K2782	L2783	E2784	A2785	L2786	F2787	T2788	K2789	V2790	L2791	T2792	GLU	GLY	L2882	S2883	R2884	D2885	V2886	T2887	V2888	V2889	W2890	I2741	I2742	V2743	Q2744	R2745	V2746	Y2747
A2687	P2688	L2689	E2690	A2691	P2692	D2693	S2694	L2695	R2696	L2697	K2698	L2699	S2700	A2701	N2702	S2703	T2704	R2705	P2706	A2707	R2708	W2709	S2710	S2711	R2712	L2713	G2714	F2715	E2716	R2717		R2720	P2721	F2722	P2723	L2724	P2725	L2726	S2727	S2728	L2729	F2730	S2731	D2732	G2733	N2734	V2735	G2737	C2738	V2739	D2740	I2741	I2742	V2743	Q2744	R2745	V2746	Y2747			

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	198.87Å 198.87Å 200.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5198	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	C	0.52	0/132	0.97	0/200
2	B	0.74	0/340	1.24	7/460 (1.5%)
3	A	0.81	3/4843 (0.1%)	1.39	81/6557 (1.2%)
All	All	0.80	3/5315 (0.1%)	1.37	88/7217 (1.2%)

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
3	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2790	VAL	CA-CB	11.52	1.70	1.54
3	A	2789	LYS	CG-CD	5.76	1.69	1.52
3	A	3055	THR	CA-CB	-5.17	1.45	1.53

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2769	GLU	N-CA-C	-12.46	96.61	113.18
3	A	2452	ALA	CA-C-N	11.50	134.21	119.84
3	A	2452	ALA	C-N-CA	11.50	134.21	119.84
3	A	3089	ASP	N-CA-C	-11.48	101.54	114.62
3	A	2768	GLU	N-CA-C	-10.40	97.57	110.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	3072	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	C	121	0	73	10	0
2	B	335	0	262	48	0
3	A	4742	0	4783	740	0
All	All	5198	0	5118	766	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 74.

The worst 5 of 766 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:56:LEU:HD23	2:B:57:ARG:H	1.02	1.17
3:A:2604:ALA:HB1	3:A:2677:ALA:HB3	1.27	1.17
3:A:3040:ALA:HB1	3:A:3043:LEU:HD11	1.27	1.12
3:A:2691:ALA:HB1	3:A:2692:PRO:HD2	1.25	1.11
2:B:10:LEU:HD11	3:A:2566:ARG:HH21	1.12	1.10

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	
2	B	36/70 (51%)	23 (64%)	5 (14%)	8 (22%)	0	1
3	A	594/649 (92%)	372 (63%)	117 (20%)	105 (18%)	0	1
All	All	630/719 (88%)	395 (63%)	122 (19%)	113 (18%)	0	1

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	ASP
2	B	23	PRO
2	B	38	VAL
2	B	41	ASP
2	B	43	TRP

5.3.2 Protein sidechains ⓘ

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	
2	B	33/63 (52%)	26 (79%)	7 (21%)	1	6
3	A	521/572 (91%)	430 (82%)	91 (18%)	2	11
All	All	554/635 (87%)	456 (82%)	98 (18%)	2	10

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

Mol	Chain	Res	Type
3	A	2789	LYS
3	A	2946	LEU
3	A	2792	THR
3	A	2901	GLU
3	A	2991	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	3042	ASN

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Mol	Chain	Res	Type
3	A	3060	HIS
3	A	3079	ASN
3	A	3078	ASN
3	A	2779	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 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

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.