



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:53 PM GMT

PDB ID : 1MJE
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

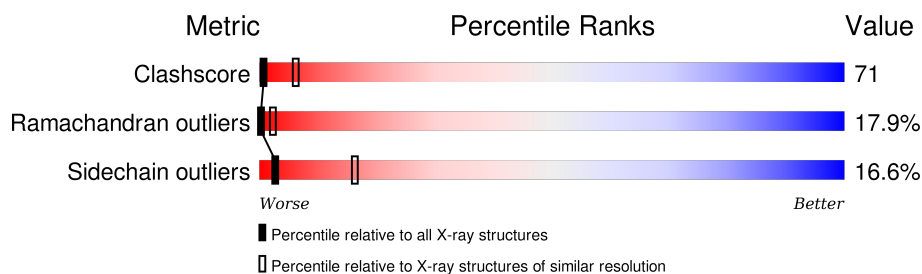
1 Overall quality at a glance

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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	6	
2	B	70	
3	A	649	

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			

K3098	L3099	I3100	H3101	V3102	L3103	P3108	K3109	W3110	SER	THR	PRO	ASN	E3030	D3031	I3032	K3033	P3034	R3035	V3036	L3037	I3038	A3039	A3040	S3041	N3042	L3043	Q3044	C3045	E3048	S3049	T3050	S3051	G3052	V3053	P3054	T3055	L3056	F3057	A3058	C3059	S3062	I3063	E3070	A3071	Y3072	F3073	Q3074	E3075	K3076	V3077	N3078	N3079	L3080	K3081	H3082	A3083	I3084	E3085	N3086	I3087	D3089	T3090	F3091	Y3092	K3093	E3096	K3097	L2964	L2965	V2966	Y2967	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	V2997	V2998	S2999	V3000	V3001	K3002	P3003	I3004	G3005	L3006	A3007	P3008	L3009	V3010	Y3011	L3012	S3013	D3014	L3017	N3018	L3019	L3020	V3021	F3024	L3028	N3029	L2749	Q2750	W2751	V2752	E2753	K2754	T2755	V2756	S2757	G2758	L2759	Y2760	I2761	F2762	R2763	S2764	E2765	R2766	E2767	E2768	E2769	K2770	E2771	A2772	L2773	R2774	F2775	A2776	Q2779	Q2780	K2781	K2782	L2783	E2784	A2785	L2786	F2787	T2788	K2789	V2790	H2791	T2792	GLY	GLY	L2882	S2883	R2884	D2885	V2886	T2887	T2888	V2889	W2890	K2891	L2892	R2893	V2894	E2895	S2896	L2687	P2688	L2689	E2690	A2691	P2692	D2693	S2694	L2695	R2696	L2697	K2698	L2699	S2700	A2701	N2702	S2703	T2704	R2705	P2706	A2707	R2708	W2709	H2710	S2711	R2712	L2713	G2714	F2715	F2716	R2717	P2721	F2722	P2723	L2724	P2725	L2726	S2727	L2728	K2729	H2730	F2731	S2731	D2732	G2733	G2734	N2735	V2736	G2737	C2738	V2739	D2740	I2741	I2742	V2743	Q2744	R2745	V2746	Y2747	P2748
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.96	1/132 (0.8%)	0.85	0/200
2	B	0.66	0/340	0.88	1/460 (0.2%)
3	A	0.66	2/4843 (0.0%)	0.92	10/6557 (0.2%)
All	All	0.67	3/5315 (0.1%)	0.92	11/7217 (0.2%)

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	7.32	1.70	1.54
1	C	501	DT	OP3-P	-6.11	1.53	1.61
3	A	2789	LYS	CG-CD	5.09	1.69	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3005	GLY	N-CA-C	-8.10	92.84	113.10
3	A	2889	VAL	CB-CA-C	-6.88	98.32	111.40
3	A	2458	PRO	N-CA-CB	5.79	110.25	103.30
3	A	2741	ILE	CB-CA-C	-5.75	100.10	111.60
3	A	2905	LEU	CA-CB-CG	-5.63	102.34	115.30

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	46	0
3	A	4742	0	4783	706	0
All	All	5198	0	5118	730	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 730 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	2
All	All	630/719 (88%)	395 (63%)	122 (19%)	113 (18%)	0	2

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%)	27 (82%)	6 (18%)	2	12
3	A	521/572 (91%)	435 (84%)	86 (16%)	3	16
All	All	554/635 (87%)	462 (83%)	92 (17%)	3	16

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2731	SER
3	A	2749	LEU
3	A	3078	ASN
3	A	2732	ASP
3	A	2741	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	2945	GLN

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Mol	Chain	Res	Type
3	A	2956	GLN
3	A	3060	HIS
3	A	2779	GLN
3	A	3042	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.