



wwPDB X-ray Structure Validation Summary Report

Jan 31, 2016 – 08:08 PM GMT

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
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)
Xtrriage (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

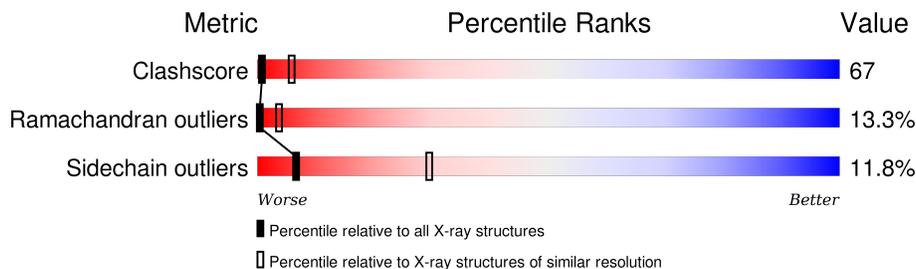
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)

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	A	70	
1	C	70	
2	B	817	
2	D	817	

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

E3094	E3095	E3096	E3097	E3098	E3099	E3100	E3101	E3102	E3103	E3104	E3105	E3106	E3107	E3108	E3109	E3110	E3111	E3112	E3113	E3114	E3115	E3116	E3117	TRP	SER	THR	PRO	ALA	ASN	LYS	ASP	PRO	THR	ARG	GLU	PRO	TYR	PRO	ALA	T3064	F3066	A3067	G3068	N3069	F3070	S3071	H3081	F3082	Q3083	E3084	R3085	V3086	T3087	N3088	N3089	K3090	H3091	A3092	I3093		
L3026	H3027	L3028	L3029	V3030	V3031	K3032	F3033	G3034	L3035	D3036	L3037	M3038	E3039	D3040	I3041	K3042	P3043	R3044	V3045	L3046	I3047	A3048	A3049	S3050	N3051	W3054	R3055	P3056	E3057	S3058	T3059	S3060	R3061	V3062	P3063	T3064	L3065	F3066	G3068	N3069	F3070	S3071	H3081	F3082	Q3083	E3084	R3085	V3086	T3087	N3088	N3089	K3090	H3091	A3092	I3093						
E2960	T2961	L2966	V2967	S2968	S2970	E2971	T2972	L2973	L2974	Q2975	Q2978	A2913	P2979	E2980	E2981	L2982	L2983	P2984	F2985	S2986	K2987	L2988	S2988	D2990	P2991	A2992	F2993	Q2994	P2996	S2998	E2999	V3000	D3001	V3002	V3005	V3007	S3008	V3009	V3010	K3011	P3012	G3013	L3014	L3015	A3016	P3017	L3018	V3019	V3020	L3021	S3022	E3024									
V2899	K2900	L2901	R2902	V2903	T2904	S2905	Y2906	K2907	K2908	R2909	E2910	K2911	S2912	A2913	L2914	L2915	S2916	I2917	M2918	R2919	P2920	S2921	S2922	L2924	P2925	S2926	L2927	L2928	L2929	E2930	G2931	Q2932	R2933	Y2934	R2935	L2936	Y2937	H2938	L2939	S2940	V2941	S2942	K2943	S2944	N2946	E2949	M2950	P2951	S2952	I2953	Q2954	L2955	T2956	A2957	K2959						
K2779	E2780	A2781	L2782	R2783	F2784	ALA	GLU	HIS	GLU	ALA	GLN	GLN	GLN	GLN	GLN	GLN	LEU	PHE	THR	LYS	LEU	VAL	L2738	F2739	S2740	D2741	G2742	G2743	N2744	V2745	G2746	C2747	V2748	D2749	V2750	I2751	E2752	Q2753	R2754	V2755	Y2756	P2757	L2758	Q2759	V2760	V2761	E2762	K2763	T2764	V2765	S2766	G2767	S2768	Y2769	R2772	N2773	E2774	R2775	E2776	A2777	E2778
T2652	D2653	G2654	W2655	Y2656	A2657	V2658	K2659	L2662	D2663	P2664	P2665	L2666	L2667	A2668	L2669	V2670	K2671	S2672	G2673	R2674	L2675	T2676	V2677	G2678	K2679	K2680	L2681	I2682	T2683	Q2684	G2685	A2686	E2687	L2688	V2689	G2690	S2691	P2692	D2693	A2694	P2697	L2698	P2701	L2704	R2705	L2706	K2707	I2708	S2709	A2710	N2711	S2712	T2713	A2714	P2715						
A2716	R2717	W2718	H2719	S2720	K2721	ALA	F2724	F2725	H2726	R2729	P2730	F2731	P2732	L2733	P2734	L2735	S2736	S2737	L2738	H2739	S2740	D2741	G2742	G2743	N2744	V2745	G2746	C2747	V2748	D2749	V2750	I2751	E2752	Q2753	R2754	V2755	Y2756	P2757	L2758	Q2759	V2760	V2761	E2762	K2763	T2764	V2765	S2766	G2767	S2768	Y2769	R2772	N2773	E2774	R2775	E2776	A2777	E2778				
GLN	ASP	ALA	SER	ASP	PRO	GLU	HIS	LEU	GLU	THR	CYS	PHE	SER	GLU	GLU	GLN	LEU	ARG	ALA	LEU	ASN	ASN	TYR	ARG	GLN	MET	LEU	SER	ASP	LYS	LYS	GLN	ALA	ARG	ILE	GLN	SER	GLU	PHE	ARG	LYS	ALA	LEU	LEU	GLU	ALA	ALA	LYS	GLU	GLU	GLY	S2892	R2893	D2894	V2896	S2896	T2897	V2898			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	5
2	D	585/817 (72%)	391 (67%)	122 (21%)	72 (12%)	0	5
All	All	1252/1774 (71%)	814 (65%)	272 (22%)	166 (13%)	0	4

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%)	2 8
1	C	41/63 (65%)	33 (80%)	8 (20%)	2 8
2	B	517/721 (72%)	459 (89%)	58 (11%)	7 32
2	D	517/721 (72%)	459 (89%)	58 (11%)	7 32
All	All	1116/1568 (71%)	984 (88%)	132 (12%)	6 29

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 will therefore be empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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