



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 02:04 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 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/ValidationPDFNotes.html>

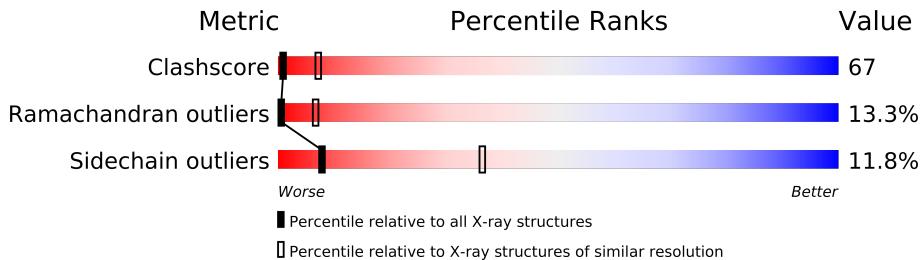
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbitiy : 4.02b-467
Mogul : 1.15 2013
Xtriaage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance (i)

The reported resolution of this entry is 3.40 Å.

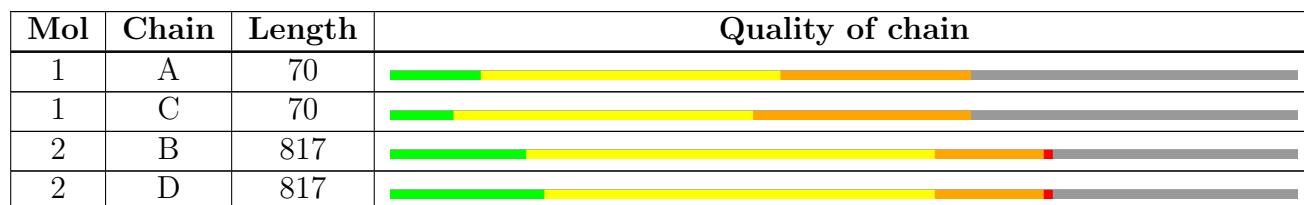
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10092 atoms, of which 0 are hydrogen and 0 are deuterium.

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	A	45	Total C N O 380 235 59 86	0	0	0
1	C	45	Total C N O 380 235 59 86	0	0	0

- Molecule 2 is a protein called breast cancer susceptibility.

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

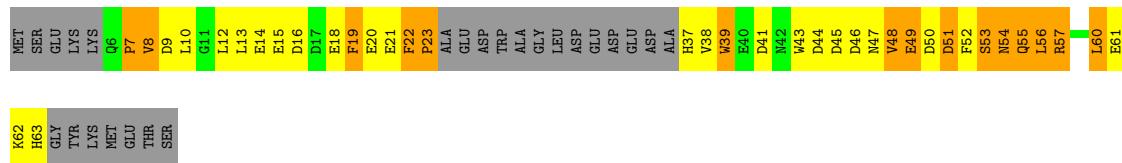
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

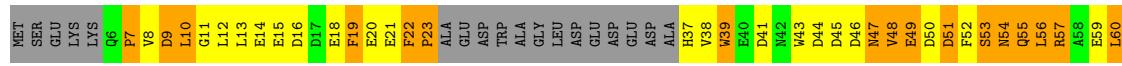
- Molecule 1: Deleted in split hand/split foot protein 1

Chain A:



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

Chain C:



- Molecule 2: breast cancer susceptibility

Chain B:



GLN	R2645	S2709
LEU	V2646	A2710
PRO	D2647	N2711
ARG	T2648	S2712
N3088	E2776	R2713
SER	R2777	R2714
K3089	E2776	R2715
SER	R2777	P2778
K3090	E2777	R2716
PRO	R2778	R2717
H3091	E2778	R2717
C3025	E2779	R2718
I3093	E2779	R2719
L3094	E2780	R2720
N3095	E2780	R2721
I3096	E2781	R2722
D3097	E2782	R2723
V3031	E2783	R2724
T3098	E2784	R2725
F3032	E2784	R2726
F3033	E2785	R2727
F3100	E2785	R2728
K3101	E2786	R2729
G3034	E2786	R2730
I3035	E2787	R2731
V3036	E2787	R2732
L3037	E2788	R2733
K3038	E2788	R2734
E3039	E2789	R2735
P2978	E2789	R2736
P2979	E2790	R2737
L2972	E2790	R2738
I2973	E2791	R2739
R2974	E2791	R2740
S2975	E2792	R2741
K2976	E2792	R2742
V2977	E2793	R2743
S2978	E2793	R2744
P2979	E2794	R2745
R2979	E2794	R2746
L2980	E2795	R2747
E2981	E2795	R2748
V2982	E2796	R2749
I2983	E2796	R2750
M2984	E2797	R2751
P2984	E2797	R2752
P2985	E2798	R2753
F2985	E2798	R2754
R2986	E2799	R2755
S2986	E2799	R2756
K2987	E2799	R2757
L2988	E2800	R2758
S2989	E2800	R2759
I2990	E2800	R2760
K3111	E2801	R2761
S3044	E2801	R2762
K3112	E2802	R2763
V3045	E2802	R2764
T3107	E2803	R2765
I3108	E2804	R2766
E3102	E2804	R2767
A3103	E2805	R2768
E3104	E2805	R2769
K3105	E2806	R2770
N3039	E2806	R2771
K3106	E2807	R2772
R3040	E2807	R2773
T3041	E2808	R2774
E3108	E2808	R2775
Q3109	E2809	R2776
V3110	E2809	R2777
E3104	E2810	R2778
K3104	E2810	R2779
S3043	E2811	R2780
I3111	E2811	R2781
R3043	E2812	R2782
K3111	E2812	R2783
S3044	E2813	R2784
K3112	E2813	R2785
V3045	E2814	R2786
T3046	E2814	R2787
I3113	E2815	R2788
D3114	E2815	R2789
A3047	E2816	R2790
S3115	E2816	R2791
A3048	E2817	R2792
P3049	E2817	R2793
K3116	E2818	R2794
S3050	E2818	R2795
K3117	E2819	R2796
TRP	D2990	E2820
SER	P2991	E2821
THR	A2992	E2822
D3114	A2992	E2823
S3115	A2992	E2824
P3116	A2992	E2825
K3117	A2992	E2826
TRP	N3051	E2827
SER	P2993	E2828
THR	N3054	E2829
PRO	R3055	E2829
ASN	P3056	E2830
LYS	E3057	E2830
ASP	P2995	E2831
ASP	S3058	E2831
PRO	P2996	E2832
THR	S3060	E2832
ARG	R3061	E2833
GLU	V3062	E2833
PRO	P3063	E2834
TYR	T3064	E2834
PRO	L3065	E2835
ALA	P3066	E2835
SER	A3067	E2836
GLN	G3068	E2836
CYS	N3069	E2837
SER	F3070	E2838
ALA	S3071	E2838
SER	V3072	E2839
ASP	F3073	E2839
LEU	I3073	E2840
ALA	A3074	E2840
SER	H3081	E2841
GLY	F3082	E2841
Q3083	P3083	E2842
GLY	E3084	E2842

- Molecule 2: breast cancer susceptibility

Chain D:

4 Data and refinement statistics (i)

Xtriage (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.	Xtriage
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($^{\circ}$)	Ideal($^{\circ}$)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4666	0	4694	652	0
2	D	4666	0	4694	629	0
All	All	10092	0	10000	1356	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 67.

The worst 5 of 1356 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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%)	1 9
2	D	585/817 (72%)	391 (67%)	122 (21%)	72 (12%)	1 8
All	All	1252/1774 (71%)	814 (65%)	272 (22%)	166 (13%)	0 7

5 of 166 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	47	ASN
1	A	51	ASP

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Mol	Chain	Res	Type
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 10
1	C	41/63 (65%)	33 (80%)	8 (20%)	2 10
2	B	517/721 (72%)	459 (89%)	58 (11%)	9 39
2	D	517/721 (72%)	459 (89%)	58 (11%)	9 39
All	All	1116/1568 (71%)	984 (88%)	132 (12%)	8 36

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 chains 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

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.