WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

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
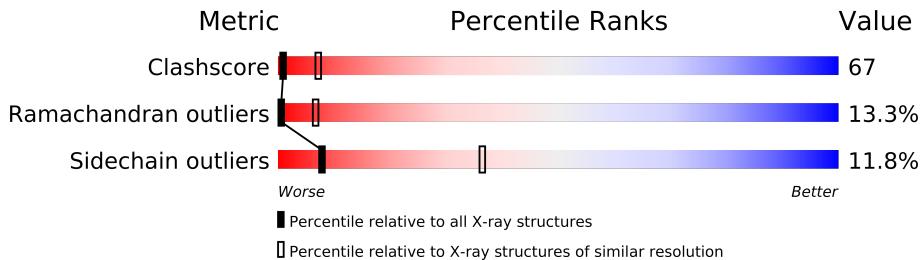
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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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	Percentile Ranks	Value
Clashscore		67
Ramachandran outliers		13.3%
Sidechain outliers		11.8%

Worse / Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

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.

Mol	Chain	Length	Quality of chain
1	A	70	
1	C	70	
2	B	817	
2	D	817	
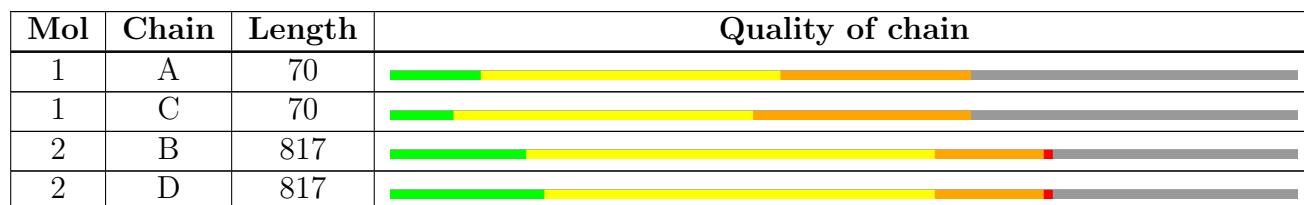
2   Entry composition   ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10092 atoms, of which 0 are 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	0	0	0
			380	235	59	86			
1	C	45	Total	C	N	O	0	0	0
			380	235	59	86			

- Molecule 2 is a protein called breast cancer susceptibility.

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

3 Residue-property plots ⓘ

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.
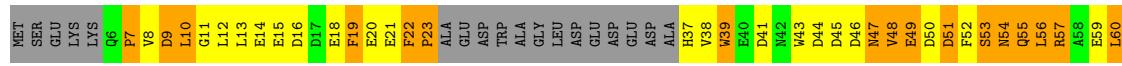
Note EDS was not executed.

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

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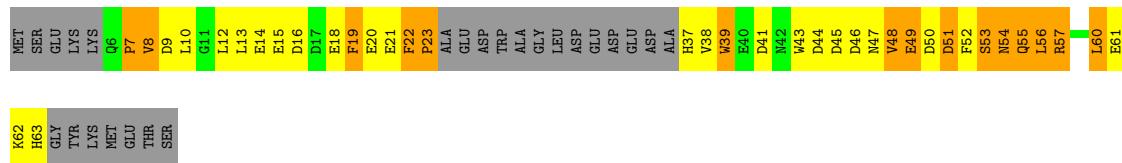
- Molecule 1: Deleted in split hand/split foot protein 1

Chain C:

- Molecule 2: breast cancer susceptibility

Chain B:

• 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 ⓘ

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	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(^{o})	Ideal(^{o})
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 ⓘ

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 ⓘ

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 ⓘ

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 ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

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.