



# 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](mailto: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.

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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

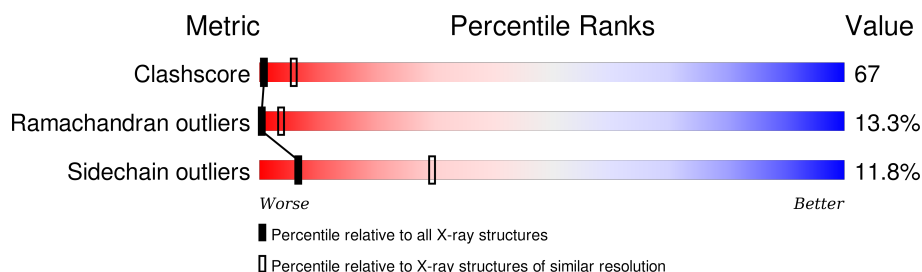
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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  $\geq 3$ , 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
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.

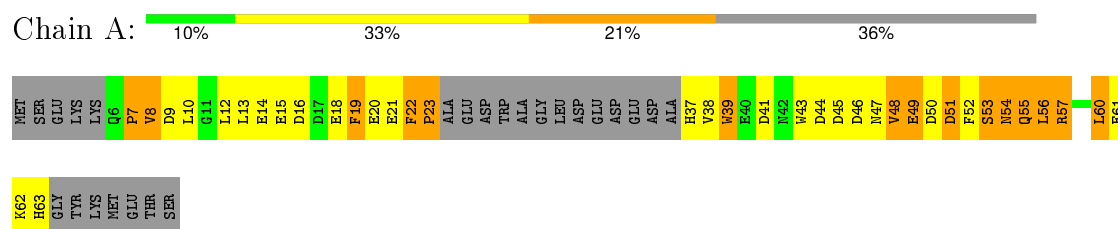
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	591	Total	C	N	O	S	0	0	0
			4666	2984	805	862	15			
2	D	591	Total	C	N	O	S	0	0	0
			4666	2984	805	862	15			

### 3 Residue-property plots

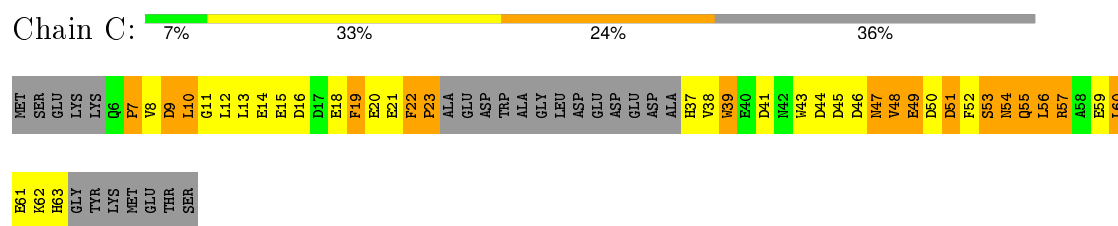
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

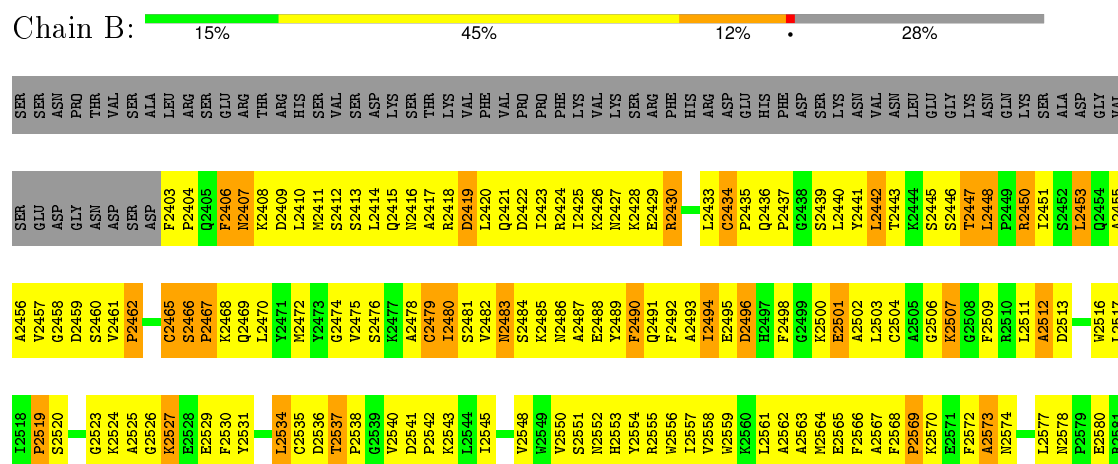
- Molecule 1: Deleted in split hand/split foot protein 1



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



- Molecule 2: breast cancer susceptibility



V2582	V2645	S2709	R2772	ALA	S2892	I2953	L3018	R3085	GLN
L2583	V2646	A2710	R2773	GLU	R2893	Q2954	V3019	V3086	LEU
L2584	D2647	N2711	N2773	LEU	V2894	L2955	Y3020	T3087	PRO
Q2585	T2648	S2712	E2776	TYR	S2896	T2956	L3021	N3088	ARG
L2586	L2651	T2713	E2777	ALA	S2897	A2957	D3022	M3089	ASN
K2587	L2652	R2714	E2778	ALA	T2897	T2958	S3023	K3090	VAL
Y2588	D2653	P2715	K2779	VAL	V2898	K2959	E3024	H3091	SER
R2589	G2654	A2716	K2780	GLN	V2899	T2960	C3025	A3092	PRO
Y2590	G2655	R2717	E2781	ASP	K2900	L2961	L3026	L3093	ALA
D2591	Y2656	H2718	A2782	ASP	L2901	L2966	H3027	E3094	LEU
V2592	A2657	H2719	L2783	SER	R2902	P2967	L3028	N3095	ARG
E2593	V2658	S2720	R2783	ASP	V2903	V2968	L3029	I3096	GLU
		K2721	F2784	PRO	T2904	S2969	V3030	D3097	ARG
		L2722	ALA	GLU	S2905	S2970	V3031	T3098	THR
N2596	K2659	L2723	GLU	HIS	Y2906	E2971	K3032	F3099	ARG
S2597	A2660	F2724	ALA	LEU	K2907	S2972	F3033	Y3100	THR
S2598	L2662	H2725	GLN	GLU	K2908	T2972	L3034	K3101	HIS
R2599	D2663	R2726	THR	THR	R2909	L2973	I3035	E3102	VAL
S2600	P2664		LYS	CYS	E2910	Q2974	D3036	A3103	SER
A2601	P2665		LYS	PHE	R2911	Q2975	L3041	E3104	ASP
L2602	P2666	R2729	LEU	ARG	S2912		K3042	I3108	LYS
K2603	L2666	P2730	LEU	THR	A2913	Q2978	N3038	Q3109	VAL
K2604	L2667	F2731	GLU	ALA	L2914	P2979	E3039	L3110	PHE
L2605	A2668	P2732	ALA	GLU	L2915	R2980	D3040	K3112	VAL
L2606	L2669	L2733	LEU	GLN	R2916	E2981	I3041	L3113	PRO
E2607	V2670	P2734	PHE	LEU	L2917	L2982	P3043	D3114	PHE
R2608	K2671	L2735	THR	ARG	K2918	L2983	V3044	G3115	PRO
D2609	S2672	S2736	LYS	ALA	R2919	P2984	V3045	D3116	LYS
D2610	G2673	S2737	VAL	LEU	F2985	L2987	L3046	S3115	VAL
T2611	R2674	L2738	HIS	ASN	S2921	K2987	I3047	P3116	VAL
A2612	L2675	F2739	THR	ASN	R2922	L2988	A3048	K3117	ARG
L2613	T2676	S2740	GLU	TYR	D2923	S2989	A3049		SER
K2614	V2677	D2741	LEU	ARG	L2924	D2990	V3050	TRP	THR
L2615	G2678	G2742	LYS	GLN	P2925	P2991	N3051		THR
L2616	K2680	N2744	HIS	LEU	L2927	A2992		P3054	PRO
V2620	L2681	V2745	GLU	SER	L2928	F2993	R3055	P3056	ASN
S2621	I2682	G2746	GLU	ASP	T2929	Q2994	E3057	S3058	LYS
D2622	T2683	C2747	ASP	LYS	E2930	P2995	S3059	T3059	ASP
L2623	G2684	V2748	ILE	GLN	Q2931	P2996	S3060	R3061	THR
L2624	Q2685	D2749	ALA	GLN	R2932	C2997	V3062	V3063	ARG
S2625	A2686	V2750	ALA	ARG	R2933	S2998	L3064	T3065	PRO
L2626	E2687	I2751	ARG	ILE	Y2934	E2999	G3066	G3068	ALA
S2627	L2688	V2752	ARG	GLN	R2935	V3000	A3067	G3069	THR
THR	V2689	Q2753	VAL	SER	L2936	D3001	F3067	R3069	CYS
ASN		R2754	LEU	GLU	Y2937	V3002	S3070	S3071	SER
VAL		V2755	SER	PHE	H2938		L3070	S3072	ALA
SER		P2756	ARG	ARG	L2939	V3005	A3071	F3073	ASP
GLU		T2757	ALA	LYS	S2940	V3007	G3068		LEU
THR		L2758	THR	ALA	V2941	S3008		H3081	ALA
SER		Q2759	ANG	LEU	S2942			F3082	SER
GLY		W2760	GLU	GLU	R2943			K3083	GLY
SER		V2761	GLN	GLN	S2944				VAL
LYS		E2762	ALA	ALA	R2945				
ALA		K2763	VAL	VAL	L2946				
LYS		P2701	GLU	LYS					
SER		T2704	LYS	LYS					
SER		V2705	GLU	GLU					
GLU		R2706	LEU	GLU					
ASP		G2767	GLN	GLY					
SER		S2768	ASP	ASP					
ASN		Y2769	GLY	LEU					

• Molecule 2: breast cancer susceptibility

Chain D: 17% 43% 12% 28%

SER	SER	S2459	K2524	V2588
SER	GLU	S2460	A2525	R2589
ASN	ASP	V2461	G2526	R2590
PRO	GLY	P2462	K2527	I2591
THR	ASN	L2463	E2528	V2592
VAL	ASP	A2464	E2529	E2593
SER	SER	C2465	F2530	
SER	ASP	S2466	Y2531	N2596
ALA	ASP	P2467		S2597
LEU	F2403	K2408		R2598
ARG	P2404	D2409		S2599
ARG	Q2405	Q2406		R2600
GLU	P2406	L2407		S2601
ARG	L2407	L2407		L2602
THR	K2408	K2408		K2603
ARG	D2409	D2409		R2604
HIS	L2410	L2410		L2605
SER	N2411	S2476		L2606
VAL	S2412	T2477		S2607
SER	S2413	A2478		R2608
ASP	L2414	C2479		D2609
LYS	Q2415	S2481		T2610
SER	N2416	V2482		D2612
THR	A2417	L2483		A2613
LYS	R2418	S2484		K2614
VAL	D2419	K2485		T2615
PHE	L2420	L2486		L2616
VAL	Q2421	A2487		
PRO	D2422	E2488		V2620
PRO	L2423	P2489		S2621
PHE	D2424	V2490		D2622
LYS	L2425	Q2491		L2623
VAL	L2426	F2492		S2625
LYS	N2427	A2493		T2626
ARG	E2428	L2494		K2613
SER	R2429	E2495		L2614
PHE	R2430	D2496		L2616
HIS	L2433	R2497		V2620
ARG	C2434	F2498		S2621
ASP		K2499		D2622
GLU	P2437	L2500		L2623
HIS	Q2438	E2501		S2625
PHE	S2439	A2502		L2626
ASP	L2440	L2503		S2627
SER	Y2441	C2504		THR
LYS	L2442	A2505		ASN
ASN	T2443	G2506		VAL
ASN	R2444	R2507		SER
LEU	S2445			ALA
GLY	S2446			SER
GLY	T2447			GLU
LYS	L2448			ASP
ASN	P2449			SER
GLN	R2450			THR
LYS	L2451			GLY
SER	S2452			SER
ALA	L2453			GLU
ASP	P2454			ASP
GLY	V2457			SER
VAL				ASN

E3094	M3095	I3096	D3097	F3098	F3099	Y3100	K3101	E3102	A3103	E3104	K3105	K3106	L3107	I3108	Q3109	V3110	L3111	K3112	G3113	D3114	S3115	P3116	K3117	TRP	SER	THR	PRO	ASN	LYS	ASP	PRO	THR	ARG	GLU	PRO	TYR	P3063	T3064	L3065	F3066	G3067	M3068	F3070	S3071	H3081	Q3082	G3083	E3084	R3085	V3086	T3087	M3088	N3089	K3090	H3091	A3092	I3093																																																																																				
C3025	L3026	H3027	L3028	L3029	V3030	V3031	K3032	F3033	G3034	I3035	D3036	L3037	M3038	E3039	D3040	I3041	P3042	R3043	V3044	L3045	L3046	I3047	A3048	A3049	S3050	N3051	W3054	R3055	P3056	E3057	S3058	T3059	S3060	R3061	V3062	P3063	T3064	L3065	F3066	G3067	M3068	F3070	S3071	H3081	Q3082	G3083	E3084	R3085	V3086	T3087	M3088	N3089	K3090	H3091	A3092	I3093																																																																																					
E2960	T2961	L2966	P2967	V2968	S2969	S2970	E2971	T2972	L2973	L2974	Q2975	Q2978	P2979	P2980	E2981	L2982	L2983	P2984	F2985	S2986	K2987	L2988	S2989	D2990	P2991	A2992	F2993	Q2994	P2995	P2996	C2997	S2998	E2999	V3000	D3001	V3002	V3005	V3006	V3007	S3008	V3009	K3010	K3011	P3012	I3013	L3014	L3015	A3016	P3017	L3018	V3019	V3020	L3021	S3022	E3024																																																																																						
W2899	K2900	I2901	V2903	T2904	S2905	Y2906	K2907	K2908	R2909	E2910	K2911	S2912	A2913	L2914	L2915	S2916	I2917	W2918	R2919	P2920	S2921	S2922	D2923	L2924	P2925	S2926	L2927	L2928	T2929	E2930	G2931	Q2932	R2933	Y2934	R2935	L2936	Y2937	E2938	L2939	S2940	V2941	S2942	R2943	S2944	K2945	N2946	E2949	W2950	P2951	S2952	I2953	Q2954	L2955	T2956	A2957	G2958	K2959																																																																																				
GLN	ASP	ALA	SER	ASP	PRO	GLU	HIS	LEU	GLU	THR	CYS	PHE	SER	GLU	GLU	GLN	LEU	ARG	ALA	LEU	ASN	THR	TYR	ARG	GLN	MET	LEU	SER	ASP	LYS	LYS	GLN	ALA	ARG	R2933	I2934	R2935	L2936	Y2937	E2938	L2939	S2940	V2941	S2942	R2943	S2944	K2945	N2946	E2949	W2950	P2951	S2952	I2953	Q2954	L2955	T2956	A2957	G2958	K2959																																																																																		
K2779	E2780	A2781	L2782	R2783	F2784	ALA	GLU	HIS	LEU	ALA	GLN	GLN	LYS	LYS	P2730	F2731	L2732	L2733	P2734	L2735	S2736	S2737	L2738	F2739	HIS	S2740	GLU	D2741	G2742	G2743	N2744	V2745	I2751	V2752	ARG	ARG	I2753	VAL	LEU	SER	GLU	PHE	ARG	LYS	ALA	THR	LEU	GLN	ALA	VAL	HIS	S2765	G2767	S2768	Y2769	R2772	N2773	GLU	A2710	S2709	I2708	K2707	L2706	R2705	L2704	P2697	L2698	P2701	HIS	ALA	THR	LEU	VAL	S2755	V2754	Q2753	ARG	GLN	VAL	LEU	SER	GLN	ARG	S2692	S2691	G2690	V2689	L2688	V2687	L2682	C2747	GLU	ASP	LYS	T2748	V2749	L2750	ALA	ALA	G2685	Q2684	T2683	L2681	Q2679	K2680	V2677	T2676	L2675	R2674	HIS	S2673	G2672	K2671	L2670	V2669	L2668	A2668	L2667	L2666	P2665	P2664	D2663	L2662	K2659	V2658	A2657	Y2656	S2720	R2783	K2721	K2722	S2729	P2730	F2731	H2726	F2725	F2724	K2717	A2716	D2653	T2652

## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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(°)	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

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 ⓘ

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.