wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 09:08 am BST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

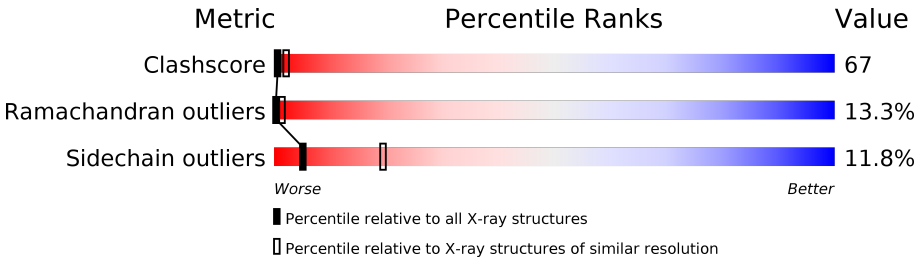
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	70	10% 33% 21% 36%
1	C	70	7% 33% 24% 36%
2	B	817	15% 45% 12% • 28%
2	D	817	17% 43% 12% • 28%

2 Entry composition (i)

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			

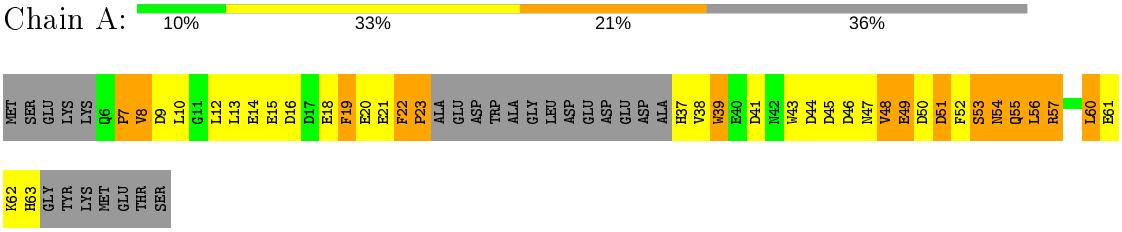
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

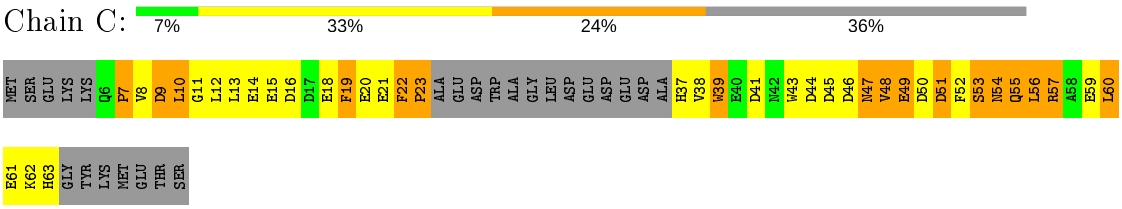
- Molecule 1: Deleted in split hand/split foot protein 1

Chain A:



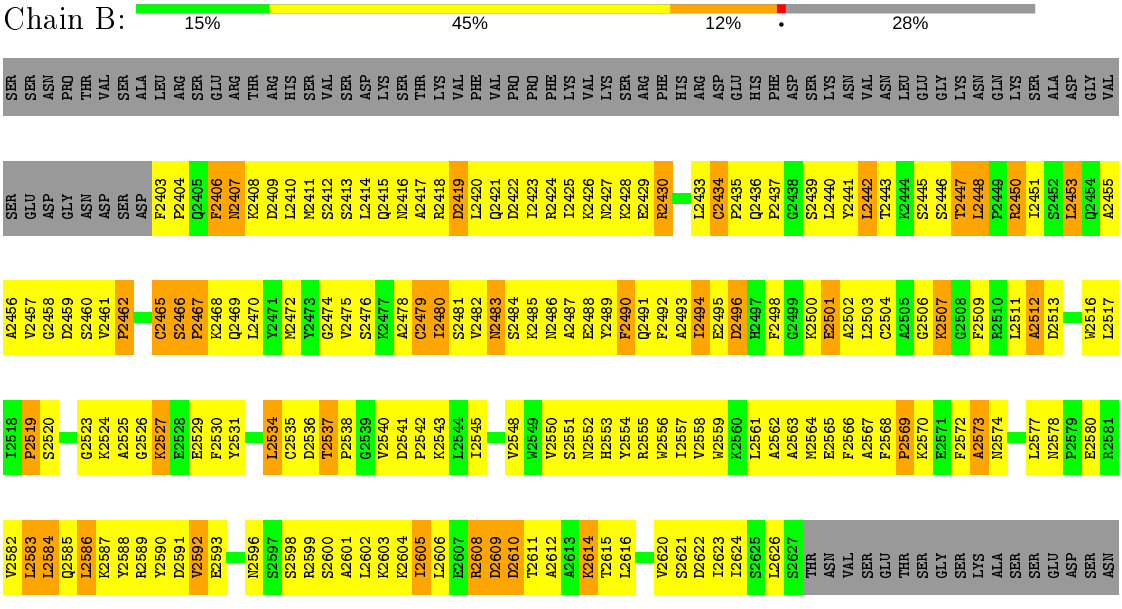
- Molecule 1: Deleted in split hand/split foot protein 1

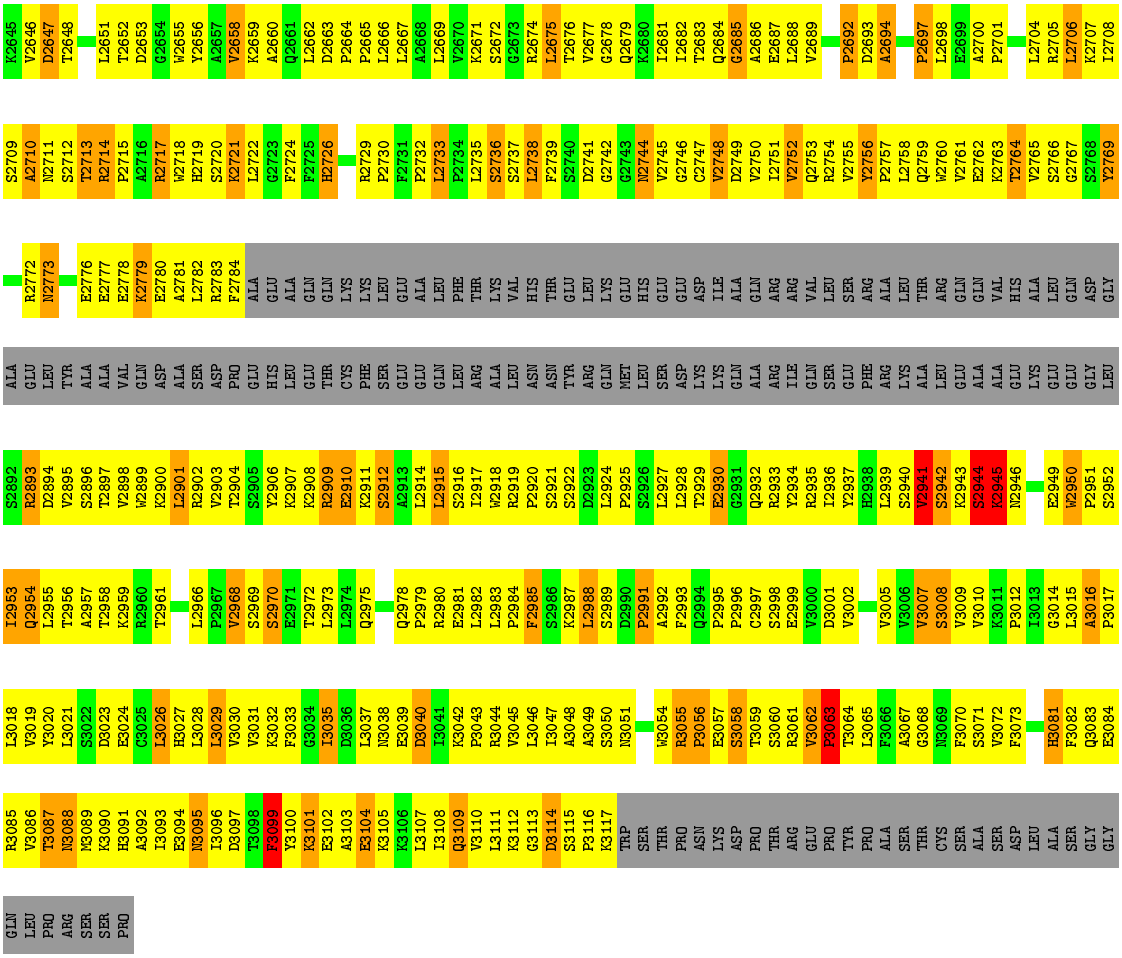
Chain C:



- Molecule 2: breast cancer susceptibility

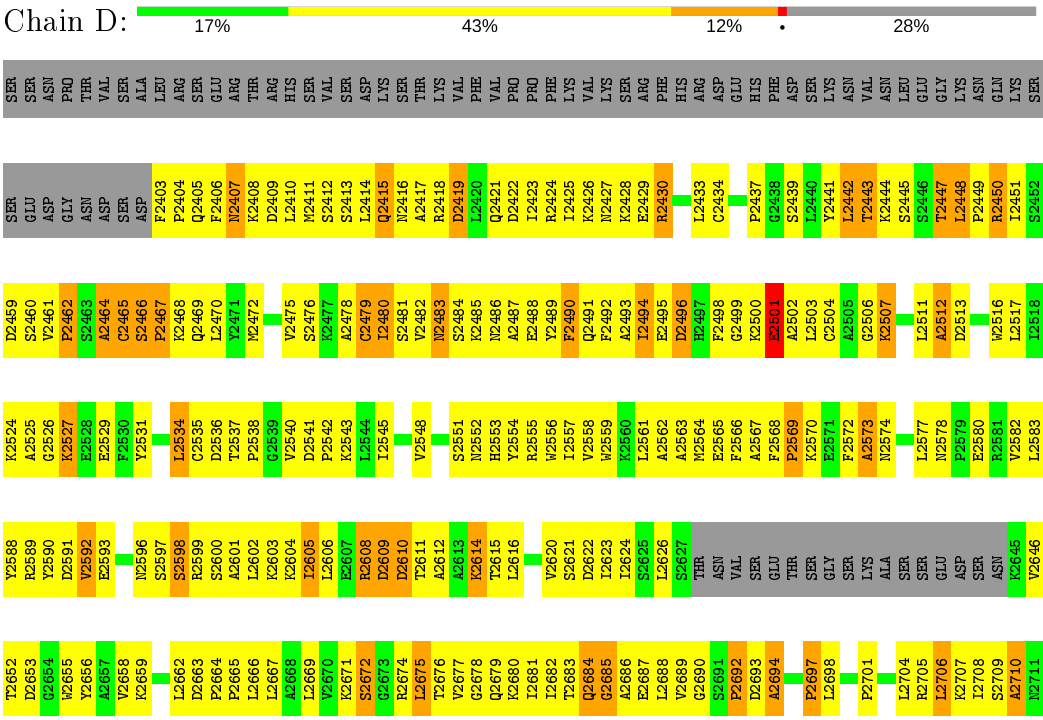
Chain B:

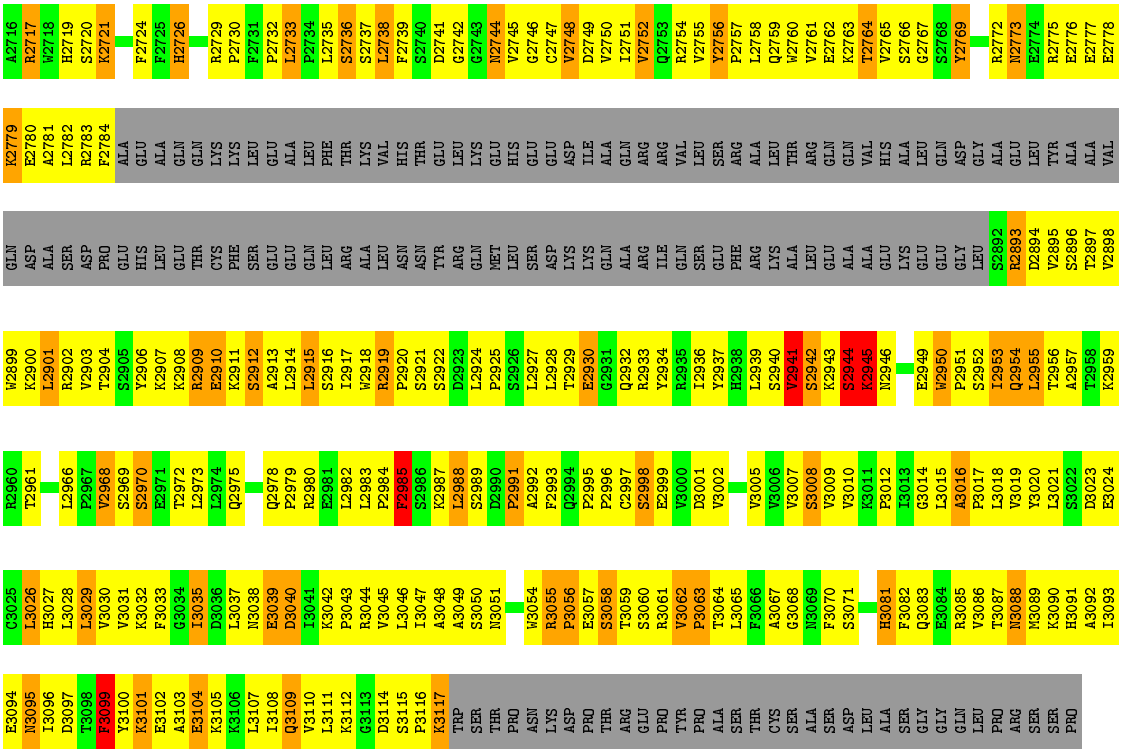




• Molecule 2: breast cancer susceptibility

Chain D:




A2716 R2717 W2718 H2719 S2720 K2721 F2724 F2725 H2726 R2729 P2730 F2731 P2732 L2733 P2734 L2735 S2736 S2737 L2738 F2739 S2740 D2741 G2742 G2743 N2744 V2745 G2746 C2747 V2748 D2749 V2750 I2751 V2752 Q2753 R2754 V2755 Y2756 P2757 L2758 Q2759 W2760 V2761 E2762 K2763 T2764 V2765 S2766 G2767 S2768 Y2769 R2772 N2773 E2774 R2775 E2776 E2777 E2778
K2779 E2780 A2781 L2782 R2783 F2784 ALA GLU ALA GLN GLN LYS LYS LEU GLU ALA LEU PHE THR LYS VAL HIS THR GLU LEU LYS GLU HIS GLU GLU ASP ILE ALA GLN ARG ARG VAL LEU SER ARG ALA LEU THR ARG GLN GLN VAL HIS ALA LEU GLN ASP GLY ALA GLU LEU TYR ALA ALA VAL
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 GLU ALA ALA GLU LYS GLU GLU GLY LEU S2892 R2893 D2894 Y2895 S2896 T2897 V2898
W2899 K2900 L2901 R2902 V2903 T2904 S2905 V2906 K2907 K2908 R2909 E2910 K2911 S2912 A2913 L2914 L2915 S2916 T2917 W2918 R2919 P2920 S2921 S2922 D2923 L2924 P2925 S2926 L2927 L2928 T2929 E2930 G2931 Q2932 R2933 Y2934 R2935 I2936 Y2937 H2938 L2939 S2940 V2941 S2942 K2943 S2944 K2945 N2946 E2949 W2950 P2951 S2952 I2953 Q2954 L2955 T2956 A2957 T2958 K2959
R2960 T2961 L2966 P2967 V2968 S2969 S2970 E2971 T2972 I2973 L2974 Q2975 Q2978 P2979 R2980 E2981 I2982 L2983 P2984 F2985 S2986 K2987 I2988 S2989 D2990 P2991 A2992 F2993 Q2994 P2995 P2996 C2997 S2998 E2999 V3000 D3001 V3002 V3005 V3006 V3007 S3008 V3009 V3010 K3011 P3012 I3013 G3014 L3015 A3016 P3017 L3018 V3019 Y3020 L3021 S3022 D3023 E3024
C3025 L3026 H3027 L3028 L3029 V3030 V3031 K3032 F3033 G3034 I3035 D3036 L3037 N3038 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 A3067 G3068 N3069 F3070 S3071 H3081 F3082 Q3083 E3084 R3085 V3086 T3087 N3088 M3089 K3090 H3091 A3092 I3093
E3094 N3095 I3096 D3097 T3098 P3099 Y3100 K3101 E3102 A3103 E3104 K3105 K3106 L3107 I3108 Q3109 V3110 I3111 K3112 G3113 D3114 S3115 P3116 K3117 THR SER THR PRO ASN LYS ASP PRO THR ARG GLU PRO TYR PRO ALA SER THR CYS SER ALA SER ASP LEU ALA SER GLY GLY GLN LEU PRO ARG SER SER PRO

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 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	3
2	D	585/817 (72%)	391 (67%)	122 (21%)	72 (12%)	0	2
All	All	1252/1774 (71%)	814 (65%)	272 (22%)	166 (13%)	0	1

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%)	1 4
1	C	41/63 (65%)	33 (80%)	8 (20%)	1 4
2	B	517/721 (72%)	459 (89%)	58 (11%)	6 22
2	D	517/721 (72%)	459 (89%)	58 (11%)	6 22
All	All	1116/1568 (71%)	984 (88%)	132 (12%)	5 19

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 molecules 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.