



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2017 – 10:31 AM EST

PDB ID : 1BRS  
Title : PROTEIN-PROTEIN RECOGNITION: CRYSTAL STRUCTURAL ANALYSIS OF A BARNASE-BARSTAR COMPLEX AT 2.0-Å RESOLUTION  
Authors : Buckle, A.M.; Schreiber, G.; Fersht, A.R.  
Deposited on : unknown  
Resolution : 2.00 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  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

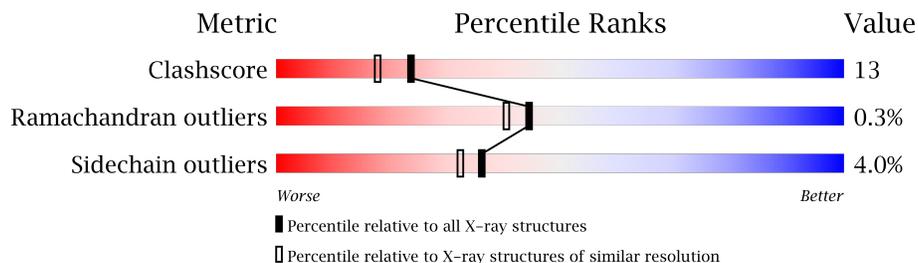
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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	110	
1	B	110	
1	C	110	
2	D	89	
2	E	89	
2	F	89	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5153 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 BARNASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	108	864	547	150	167	0	0	0
1	B	110	878	555	153	170	0	0	0
1	C	108	839	533	146	160	0	0	0

- Molecule 2 is a protein called BARSTAR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	87	695	449	112	134	0	1	0
2	E	86	665	430	103	132	0	0	0
2	F	89	699	450	116	133	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	40	ALA	CYS	CONFLICT	UNP P11540
D	82	ALA	CYS	CONFLICT	UNP P11540
E	40	ALA	CYS	CONFLICT	UNP P11540
E	82	ALA	CYS	CONFLICT	UNP P11540
F	40	ALA	CYS	CONFLICT	UNP P11540
F	82	ALA	CYS	CONFLICT	UNP P11540

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	145	145	145	0	0

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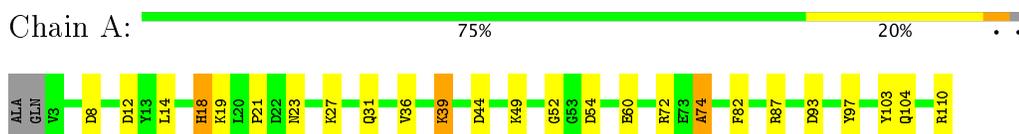
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	137	Total 137	O 137	0	0
3	C	50	Total 50	O 50	0	0
3	D	77	Total 77	O 77	0	0
3	E	64	Total 64	O 64	0	0
3	F	40	Total 40	O 40	0	0

### 3 Residue-property plots [i](#)

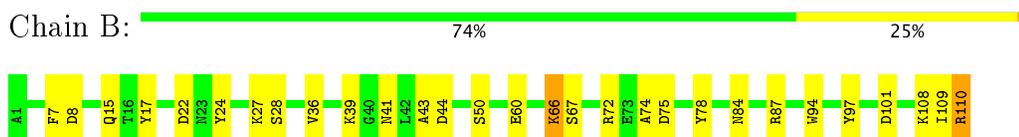
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

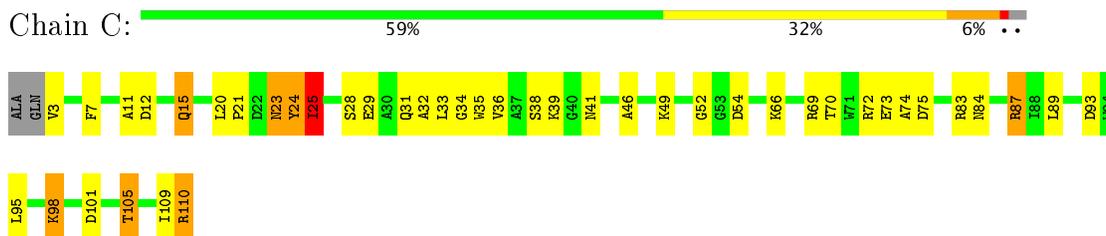
- Molecule 1: BARNASE



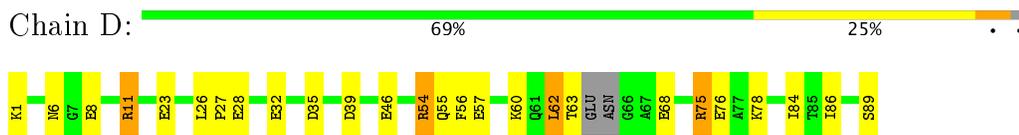
- Molecule 1: BARNASE



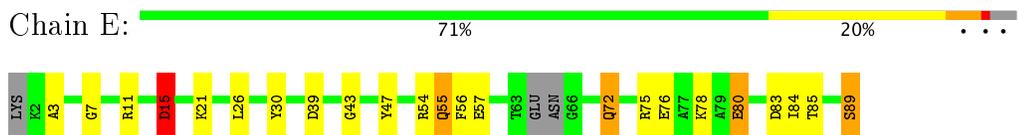
- Molecule 1: BARNASE



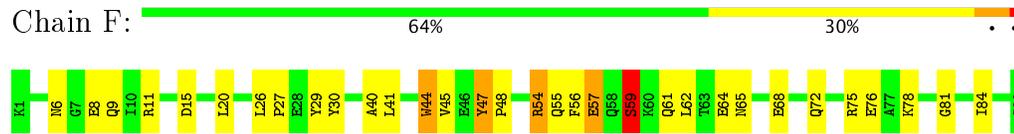
- Molecule 2: BARSTAR



- Molecule 2: BARSTAR



- Molecule 2: BARSTAR



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.25Å 43.86Å 84.71Å 90.00° 107.76° 90.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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	0.96	1/885 (0.1%)	1.86	17/1197 (1.4%)
1	B	0.84	1/899 (0.1%)	1.79	20/1216 (1.6%)
1	C	0.65	0/860	1.83	16/1168 (1.4%)
2	D	0.76	0/711	1.84	17/962 (1.8%)
2	E	0.82	1/677 (0.1%)	2.23	14/919 (1.5%)
2	F	0.73	0/712	1.91	16/966 (1.7%)
All	All	0.80	3/4744 (0.1%)	1.90	100/6428 (1.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	ARG	C-O	16.42	1.54	1.23
1	B	110	ARG	C-O	11.40	1.45	1.23
2	E	89	SER	C-O	-8.76	1.06	1.23

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	E	75	ARG	CD-NE-CZ	34.29	171.60	123.60
2	E	75	ARG	NE-CZ-NH2	21.53	131.06	120.30
2	F	75	ARG	NE-CZ-NH2	-15.00	112.80	120.30
2	E	75	ARG	NE-CZ-NH1	-14.70	112.95	120.30
2	E	15	ASP	CB-CG-OD2	-13.33	106.30	118.30

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	864	0	833	29	0
1	B	878	0	849	9	0
1	C	839	0	782	27	0
2	D	695	0	689	17	0
2	E	665	0	633	14	0
2	F	699	0	689	19	0
3	A	145	0	0	3	1
3	B	137	0	0	2	1
3	C	50	0	0	3	0
3	D	77	0	0	3	0
3	E	64	0	0	1	0
3	F	40	0	0	2	0
All	All	5153	0	4475	115	1

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 13.

The worst 5 of 115 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)
1:A:36:VAL:HB	1:A:39:LYS:CG	1.62	1.30
1:A:39:LYS:CB	1:A:39:LYS:NZ	2.10	1.14
1:A:39:LYS:CB	1:A:39:LYS:HZ2	1.63	1.10
1:A:36:VAL:HB	1:A:39:LYS:HG3	1.32	1.08
2:E:55:GLN:HA	2:E:55:GLN:HE21	1.16	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:208:HOH:O	3:B:166:HOH:O[2_555]	2.10	0.10

## 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	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	B	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
1	C	106/110 (96%)	92 (87%)	13 (12%)	1 (1%)	20	12
2	D	84/89 (94%)	80 (95%)	4 (5%)	0	100	100
2	E	82/89 (92%)	78 (95%)	4 (5%)	0	100	100
2	F	87/89 (98%)	81 (93%)	5 (6%)	1 (1%)	17	9
All	All	573/597 (96%)	541 (94%)	30 (5%)	2 (0%)	44	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	LEU
2	F	44	TRP

### 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	91/92 (99%)	90 (99%)	1 (1%)	78	82
1	B	92/92 (100%)	89 (97%)	3 (3%)	43	41
1	C	83/92 (90%)	75 (90%)	8 (10%)	10	5
2	D	72/76 (95%)	69 (96%)	3 (4%)	34	30
2	E	66/76 (87%)	63 (96%)	3 (4%)	32	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	71/76 (93%)	70 (99%)	1 (1%)	71	76
All	All	475/504 (94%)	456 (96%)	19 (4%)	36	32

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	66	LYS
1	C	98	LYS
2	E	15	ASP
1	C	38	SER
2	E	55	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	55	GLN
2	F	61	GLN
2	F	18	GLN
1	C	18	HIS
2	F	6	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

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.