



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:31 AM UTC

PDB ID : 1BNF / pdb_00001bnf
Title : BARNASE T70C/S92C DISULFIDE MUTANT
Authors : Clarke, J.; Henrick, K.; Fersht, A.R.
Deposited on : 1995-03-31
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

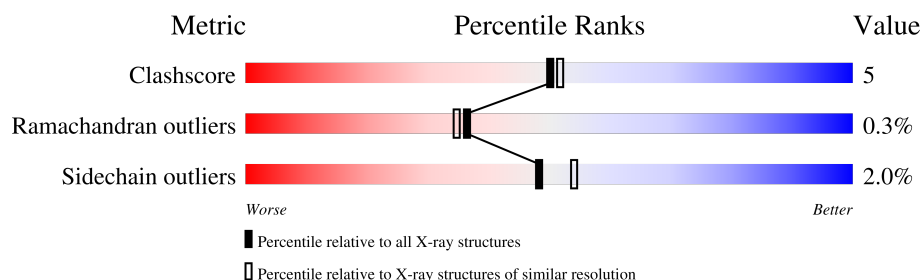
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	110	 69% 26% . .
1	B	110	 70% 25% . .
1	C	110	 69% 23% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2771 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
1	A	108	Total	C	N	O	S	0	2	0
			847	540	142	161	4			
1	B	107	Total	C	N	O	S	0	2	0
			849	537	144	164	4			
1	C	107	Total	C	N	O	S	0	2	0
			847	536	143	164	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	CYS	THR	conflict	UNP P00648
A	92	CYS	SER	conflict	UNP P00648
B	70	CYS	THR	conflict	UNP P00648
B	92	CYS	SER	conflict	UNP P00648
C	70	CYS	THR	conflict	UNP P00648
C	92	CYS	SER	conflict	UNP P00648

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		
2	B	78	Total	O	0	0
			78	78		
2	C	84	Total	O	0	0
			84	84		

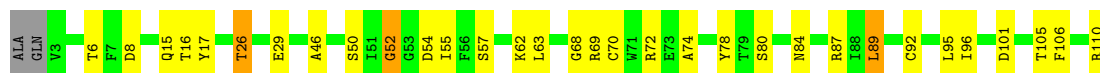
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

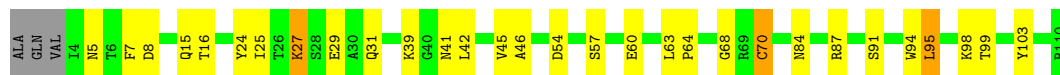
• Molecule 1: BARNASE

Chain A:  69% 26% . .



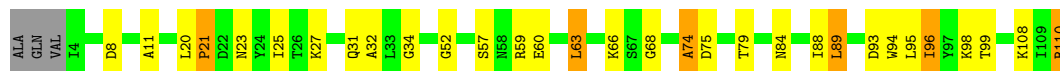
• Molecule 1: BARNASE

Chain B:  70% 25% . .



• Molecule 1: BARNASE

Chain C:  69% 23% 5% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	59.14Å 59.14Å 81.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2771	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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	1.05	0/872	2.08	24/1180 (2.0%)
1	B	1.13	0/874	2.04	24/1183 (2.0%)
1	C	1.09	0/872	2.06	24/1180 (2.0%)
All	All	1.09	0/2618	2.06	72/3543 (2.0%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ASN	OD1-CG-ND2	-11.53	111.07	122.60
1	A	57	SER	CA-C-O	-9.30	110.56	120.42
1	C	93	ASP	CA-C-O	8.66	130.16	119.95
1	C	68	GLY	N-CA-C	8.44	123.12	112.83
1	B	60	GLU	CA-CB-CG	7.95	129.99	114.10
1	B	84	ASN	CB-CG-ND2	7.57	127.75	116.40
1	B	24	TYR	CA-C-O	-7.29	112.71	120.80
1	B	41	ASN	N-CA-C	7.12	120.84	112.72
1	B	95	LEU	CA-C-O	-7.08	112.98	121.05
1	A	52	GLY	CA-C-O	-6.83	114.25	121.29
1	C	79	THR	N-CA-CB	6.79	121.97	110.49
1	A	95	LEU	CA-C-O	-6.79	112.95	120.69
1	A	16	THR	CA-C-N	6.74	131.98	120.72
1	A	16	THR	C-N-CA	6.74	131.98	120.72
1	C	75	ASP	CA-C-O	-6.68	113.44	121.05
1	B	16	THR	O-C-N	6.61	130.17	122.17
1	C	79	THR	CA-C-O	-6.54	111.16	120.51
1	B	25	ILE	CA-C-O	-6.46	114.43	121.28
1	C	23	ASN	CA-C-O	-6.37	110.78	119.12
1	B	15	GLN	CA-C-O	-6.22	112.82	119.97
1	B	16	THR	CA-C-O	-6.17	113.94	120.55
1	A	46	ALA	O-C-N	6.14	125.67	121.19
1	B	31	GLN	CA-CB-CG	-6.13	101.84	114.10
1	B	57	SER	N-CA-C	6.04	118.83	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	LEU	CA-C-O	-5.97	113.91	120.36
1	C	57	SER	CA-C-O	-5.97	113.11	119.97
1	C	59	ARG	CA-C-O	-5.96	114.24	120.55
1	B	95	LEU	N-CA-C	-5.91	100.86	110.20
1	B	54	ASP	O-C-N	5.87	129.59	122.96
1	C	95	LEU	N-CA-C	-5.86	101.81	110.48
1	C	99	THR	CA-CB-OG1	-5.85	100.83	109.60
1	C	74	ALA	CA-C-O	-5.83	114.47	120.99
1	B	5	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	17	TYR	CA-C-O	5.77	126.48	119.38
1	B	99	THR	CA-CB-OG1	-5.77	100.95	109.60
1	C	63	LEU	O-C-N	5.74	126.37	121.20
1	A	80	SER	CA-C-O	-5.70	115.34	121.38
1	A	62	LYS	CB-CG-CD	5.61	124.20	111.30
1	C	108	LYS	CA-C-O	-5.57	114.40	120.81
1	C	84	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	C	8	ASP	O-C-N	5.56	128.09	122.09
1	A	8	ASP	O-C-N	5.50	128.03	122.09
1	C	98	LYS	CB-CG-CD	-5.49	98.68	111.30
1	B	29	GLU	CG-CD-OE2	-5.47	105.81	118.40
1	A	84	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	46	ALA	N-CA-CB	-5.44	104.34	111.09
1	A	6	THR	CA-CB-OG1	-5.42	101.47	109.60
1	B	57	SER	CA-C-O	-5.39	113.77	119.97
1	C	60	GLU	CG-CD-OE1	5.39	130.80	118.40
1	A	78	TYR	CA-C-O	-5.39	114.72	120.92
1	A	87	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	C	110	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	C	21	PRO	CB-CA-C	5.33	118.00	111.12
1	B	42	LEU	CA-C-O	-5.32	115.20	120.90
1	A	26	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	72	ARG	NE-CZ-NH2	-5.28	114.44	119.20
1	C	25	ILE	CA-C-O	-5.25	115.71	121.28
1	A	54	ASP	CA-C-N	5.24	127.60	120.63
1	A	54	ASP	C-N-CA	5.24	127.60	120.63
1	A	50	SER	CA-C-O	-5.23	114.99	121.11
1	B	68	GLY	N-CA-C	5.23	118.97	112.64
1	A	101	ASP	CA-C-O	-5.19	115.02	120.32
1	B	24	TYR	O-C-N	5.19	129.27	123.19
1	C	94	TRP	N-CA-C	5.15	118.83	112.24
1	C	11	ALA	O-C-N	5.15	127.37	122.07
1	B	94	TRP	N-CA-C	5.11	118.64	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	THR	OG1-CB-CG2	5.10	119.50	109.30
1	B	8	ASP	CA-C-O	-5.08	115.47	120.70
1	A	95	LEU	N-CA-C	-5.06	101.72	109.76
1	C	66	LYS	CA-C-O	-5.04	115.80	121.40
1	A	15	GLN	O-C-N	5.02	128.09	122.22
1	A	105	THR	O-C-N	5.01	129.40	123.24

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	847	0	793	8	0
1	B	849	0	798	9	0
1	C	847	0	792	11	0
2	A	66	0	0	0	0
2	B	78	0	0	2	0
2	C	84	0	0	0	1
All	All	2771	0	2383	26	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 5.

All (26) 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:B:39:LYS:HE2	2:B:183:HOH:O	2.01	0.60
1:C:96:ILE:HG13	1:C:110:ARG:HB2	1.88	0.54
1:A:55:ILE:HD12	1:A:69:ARG:HB3	1.88	0.54
1:A:89:LEU:HD13	1:A:106:PHE:CE1	2.43	0.53
1:C:63:LEU:HD11	1:C:89:LEU:HD23	1.90	0.53
1:A:89:LEU:HD13	1:A:106:PHE:HE1	1.74	0.53
1:B:27:LYS:HE3	2:B:147:HOH:O	2.10	0.52
1:B:7:PHE:CE1	1:B:98:LYS:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LEU:HD11	1:C:89:LEU:CD2	2.46	0.45
1:C:96:ILE:CG1	1:C:110:ARG:HB2	2.46	0.45
1:C:74:ALA:HB3	1:C:88:ILE:HG22	1.99	0.45
1:B:64:PRO:HG3	1:C:34:GLY:HA2	1.98	0.44
1:A:26:THR:OG1	1:A:29:GLU:HG3	2.18	0.43
1:A:63:LEU:HD11	1:A:89:LEU:HD22	2.01	0.43
1:B:87:ARG:HG3	1:B:103:TYR:CE1	2.54	0.43
1:A:70[B]:CYS:SG	1:A:92[B]:CYS:N	2.76	0.42
1:B:95:LEU:HD11	1:C:32:ALA:O	2.19	0.42
1:C:52:GLY:HA2	1:C:74:ALA:HA	2.01	0.42
1:C:20:LEU:HA	1:C:21:PRO:HD3	1.92	0.42
1:C:96:ILE:HB	1:C:110:ARG:HB2	2.02	0.42
1:A:96:ILE:HB	1:A:110:ARG:HB2	2.01	0.41
1:A:52:GLY:HA2	1:A:74:ALA:HA	2.03	0.41
1:B:63:LEU:O	1:B:64:PRO:C	2.64	0.41
1:C:27:LYS:O	1:C:31:GLN:HG3	2.20	0.40

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)
2:C:112:HOH:O	2:C:174:HOH:O[2_654]	2.15	0.05

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	108/110 (98%)	103 (95%)	4 (4%)	1 (1%)	14	9
1	B	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
1	C	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
All	All	322/330 (98%)	309 (96%)	12 (4%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY

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	85/92 (92%)	84 (99%)	1 (1%)	63	70
1	B	89/92 (97%)	85 (96%)	4 (4%)	24	23
1	C	88/92 (96%)	87 (99%)	1 (1%)	65	73
All	All	262/276 (95%)	256 (98%)	6 (2%)	48	49

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	B	27	LYS
1	B	45	VAL
1	B	70[A]	CYS
1	B	70[B]	CYS
1	C	96	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	C	31	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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 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.