



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 10:05 AM EST

PDB ID : 1BNE
Title : BARNASE A43C/S80C DISULFIDE MUTANT
Authors : Clarke, J.; Henrick, K.; Fersht, A.R.
Deposited on : 1995-03-31
Resolution : 2.10 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 : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

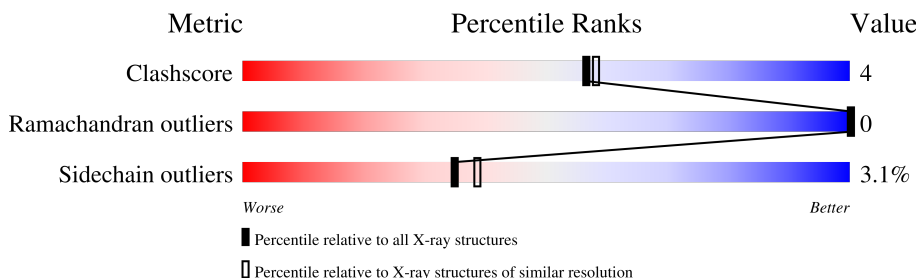
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)

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	 77% 17% . .
1	B	110	 85% 13% . .
1	C	110	 81% 16% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2770 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	3	1
			853	540	145	164	4			
1	B	108	Total	C	N	O	S	0	0	1
			838	530	143	163	2			
1	C	108	Total	C	N	O	S	0	0	1
			849	539	144	164	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	CYS	ALA	conflict	UNP P00648
A	80	CYS	SER	conflict	UNP P00648
B	43	CYS	ALA	conflict	UNP P00648
B	80	CYS	SER	conflict	UNP P00648
C	43	CYS	ALA	conflict	UNP P00648
C	80	CYS	SER	conflict	UNP P00648

- Molecule 2 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	79	Total	O	0	0
			79	79		
2	B	79	Total	O	0	0
			79	79		
2	C	72	Total	O	0	0
			72	72		

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: 




- Molecule 1: BARNASE

Chain B: 



- Molecule 1: BARNASE

Chain C: 



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	59.60Å 59.60Å 81.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.10)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2770	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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	0.92	0/880	1.62	12/1191 (1.0%)
1	B	0.91	0/859	1.44	8/1163 (0.7%)
1	C	0.91	0/870	1.63	10/1177 (0.8%)
All	All	0.91	0/2609	1.57	30/3531 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	A	110	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	A	101	ASP	CB-CG-OD1	11.33	128.50	118.30
1	C	69	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	110	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	C	44	ASP	CB-CG-OD1	8.73	126.15	118.30
1	B	12	ASP	CB-CG-OD1	7.60	125.14	118.30
1	C	108	LYS	CD-CE-NZ	-7.57	94.29	111.70
1	C	110	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	C	72	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	C	87	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	72	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	A	69	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	B	75	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	69	ARG	NE-CZ-NH1	7.16	123.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	93	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	101	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	75	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	103	TYR	CB-CG-CD1	6.05	124.63	121.00
1	B	13	TYR	CB-CG-CD1	6.00	124.60	121.00
1	B	29	GLU	OE1-CD-OE2	-5.83	116.31	123.30
1	A	86	ASP	CB-CG-OD1	5.54	123.28	118.30
1	C	13	TYR	CB-CG-CD1	5.45	124.27	121.00
1	B	13	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	13	TYR	CB-CG-CD2	5.21	124.13	121.00
1	A	103	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	C	95	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	93	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	12	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	PHE	Mainchain
1	A	79[A]	THR	Mainchain

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	853	0	790	11	0
1	B	838	0	777	4	0
1	C	849	0	800	7	0
2	A	79	0	0	0	0
2	B	79	0	0	1	0
2	C	72	0	0	0	0
All	All	2770	0	2367	22	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 4.

All (22) 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:79[A]:THR:HG22	1:A:79[A]:THR:O	1.71	0.87
1:A:79[A]:THR:O	1:A:79[A]:THR:CG2	2.31	0.77
1:A:79[B]:THR:O	1:A:80[B]:CYS:SG	2.59	0.61
1:A:89:LEU:HD13	1:A:106:PHE:HE2	1.68	0.58
1:C:101:ASP:O	1:C:104:GLN:HG3	2.03	0.58
1:A:89:LEU:HD13	1:A:106:PHE:CE2	2.41	0.56
1:A:96:ILE:HB	1:A:110:ARG:HB2	1.86	0.56
1:A:79[A]:THR:O	1:A:80[A]:CYS:HB2	2.07	0.55
1:C:27:LYS:O	1:C:31:GLN:HG3	2.12	0.50
1:C:96:ILE:CG1	1:C:110:ARG:HB2	2.42	0.50
1:B:52:GLY:HA2	1:B:74:ALA:HA	1.94	0.49
1:C:101:ASP:CG	1:C:104:GLN:HB2	2.34	0.48
1:C:52:GLY:HA2	1:C:74:ALA:HA	1.96	0.47
1:A:63:LEU:HD11	1:A:89:LEU:HD22	1.97	0.46
1:A:52:GLY:HA2	1:A:74:ALA:HA	1.97	0.46
1:C:7:PHE:CE1	1:C:98:LYS:HB2	2.50	0.46
1:B:87:ARG:HB2	1:B:99:THR:HG22	1.97	0.46
1:A:17:TYR:O	1:A:18:HIS:HB2	2.18	0.44
1:B:89:LEU:HD13	1:B:106:PHE:CE1	2.54	0.43
1:C:74:ALA:HB3	1:C:88:ILE:HG22	2.01	0.43
1:B:79:THR:HA	2:B:176:HOH:O	2.19	0.42
1:A:74:ALA:HB3	1:A:88:ILE:HG22	2.02	0.41

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	109/110 (99%)	102 (94%)	7 (6%)	0	100	100
1	B	106/110 (96%)	103 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	106/110 (96%)	101 (95%)	5 (5%)	0	100	100
All	All	321/330 (97%)	306 (95%)	15 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	87/93 (94%)	82 (94%)	5 (6%)	17	15
1	B	85/93 (91%)	82 (96%)	3 (4%)	31	34
1	C	87/93 (94%)	87 (100%)	0	100	100
All	All	259/279 (93%)	251 (97%)	8 (3%)	35	39

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	67	SER
1	A	89	LEU
1	A	96	ILE
1	A	102	HIS
1	B	5	ASN
1	B	28	SER
1	B	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	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 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.