



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:38 PM GMT

PDB ID : 1BRK
Title : BARNASE MUTANT WITH ILE 96 REPLACED BY ALA
Authors : Cramer, P.C.; Buckle, A.; Fersht, A.
Deposited on : 1995-03-09
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

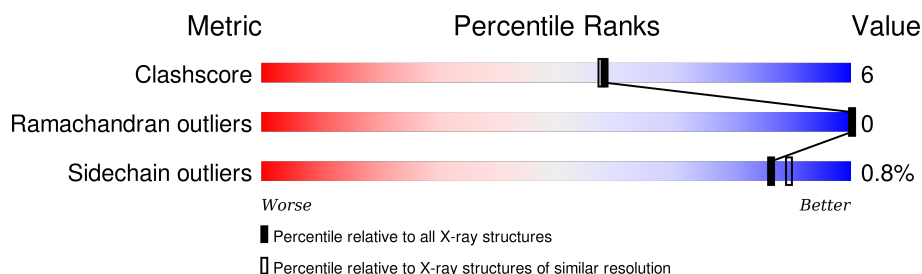
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 ≥ 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	 79% 17% . .
1	B	110	 79% 18% . .
1	C	110	 76% 21% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2875 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	0	0	0
			854	541	146	167			
1	B	108	Total	C	N	O	0	0	0
			848	539	142	167			
1	C	107	Total	C	N	O	0	0	0
			848	537	145	166			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ALA	ILE	CONFLICT	UNP P00648
B	96	ALA	ILE	CONFLICT	UNP P00648
C	96	ALA	ILE	CONFLICT	UNP P00648

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	117	Total	O	0	0
			117	117		

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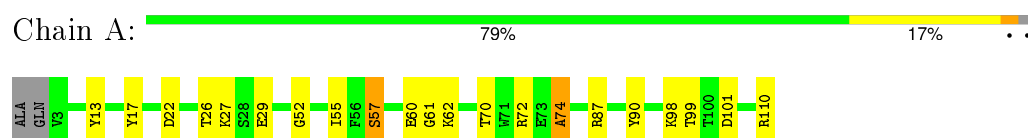
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	115	Total	O	0	0
			115	115		

3 Residue-property plots [i](#)

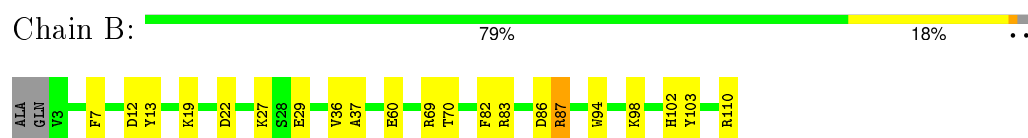
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

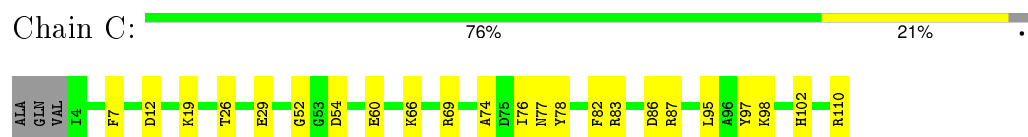
- Molecule 1: BARNASE



- Molecule 1: BARNASE



- Molecule 1: BARNASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	59.05Å 59.05Å 81.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2875	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.78	1/875 (0.1%)	1.76	16/1185 (1.4%)
1	B	0.71	0/869	1.79	19/1177 (1.6%)
1	C	0.71	0/869	1.74	16/1176 (1.4%)
All	All	0.74	1/2613 (0.0%)	1.76	51/3538 (1.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	ARG	C-OXT	10.64	1.43	1.23

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ARG	NE-CZ-NH2	12.27	126.44	120.30
1	B	13	TYR	CB-CG-CD2	-11.01	114.40	121.00
1	C	69	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	A	17	TYR	CB-CG-CD1	-9.74	115.15	121.00
1	B	110	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	B	22	ASP	CB-CG-OD1	8.50	125.95	118.30
1	B	22	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	B	87	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	B	87	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	C	78	TYR	CB-CG-CD2	8.36	126.02	121.00
1	A	57	SER	N-CA-CB	-8.07	98.39	110.50
1	A	87	ARG	CD-NE-CZ	7.85	134.59	123.60
1	A	17	TYR	CB-CG-CD2	7.77	125.66	121.00
1	A	101	ASP	CB-CG-OD1	7.72	125.25	118.30
1	B	86	ASP	CB-CG-OD1	7.66	125.19	118.30
1	B	87	ARG	NH1-CZ-NH2	-7.66	110.97	119.40
1	A	13	TYR	CB-CG-CD1	7.65	125.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	LYS	CA-CB-CG	7.64	130.21	113.40
1	B	83	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	C	78	TYR	CB-CG-CD1	-7.41	116.55	121.00
1	C	12	ASP	CB-CG-OD1	7.32	124.89	118.30
1	C	69	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	C	86	ASP	CB-CG-OD1	7.02	124.62	118.30
1	B	69	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	72	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	C	87	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	90	TYR	CB-CG-CD2	-6.64	117.01	121.00
1	B	82	PHE	CB-CG-CD2	-6.51	116.24	120.80
1	A	13	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	A	17	TYR	CA-CB-CG	-6.18	101.65	113.40
1	C	82	PHE	CB-CG-CD2	-6.14	116.50	120.80
1	B	12	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	97	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	B	13	TYR	CB-CG-CD1	5.94	124.57	121.00
1	C	60	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	C	110	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	B	94	TRP	CA-CB-CG	-5.67	102.93	113.70
1	B	13	TYR	CZ-CE2-CD2	-5.63	114.73	119.80
1	B	13	TYR	CG-CD1-CE1	-5.58	116.83	121.30
1	C	110	ARG	CD-NE-CZ	5.56	131.38	123.60
1	A	90	TYR	CB-CG-CD1	5.46	124.28	121.00
1	A	110	ARG	CA-CB-CG	5.42	125.33	113.40
1	A	99	THR	N-CA-CB	5.40	120.56	110.30
1	C	54	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	B	82	PHE	CB-CG-CD1	5.30	124.51	120.80
1	C	54	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	22	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	74	ALA	N-CA-CB	5.12	117.27	110.10
1	A	72	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	110	ARG	CA-CB-CG	5.10	124.62	113.40
1	C	95	LEU	CA-C-O	-5.07	109.45	120.10

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	854	0	811	10	0
1	B	848	0	790	9	0
1	C	848	0	804	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	90	0	0	4	5
3	B	117	0	0	7	9
3	C	115	0	0	6	7
All	All	2875	0	2405	29	17

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 6.

All (29) 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:29:GLU:HG3	3:B:187:HOH:O	1.17	1.27
1:B:37:ALA:N	3:B:177:HOH:O	1.84	1.00
1:C:102:HIS:CD2	3:C:164:HOH:O	2.24	0.91
1:C:102:HIS:HD2	3:C:164:HOH:O	1.58	0.86
1:C:66:LYS:HE2	3:C:199:HOH:O	1.75	0.85
1:C:26:THR:OG1	1:C:29:GLU:HG3	1.89	0.72
1:A:62:LYS:HD2	3:A:169:HOH:O	1.95	0.65
1:B:102:HIS:CE1	3:B:222:HOH:O	2.51	0.64
1:C:66:LYS:CE	3:C:199:HOH:O	2.40	0.63
1:A:57:SER:HB2	3:A:132:HOH:O	2.06	0.56
1:C:7:PHE:CE1	1:C:98:LYS:HB2	2.41	0.56
1:A:55:ILE:CD1	1:A:70:THR:CG2	2.85	0.54
1:A:26:THR:OG1	1:A:29:GLU:HG3	2.08	0.54
1:B:36:VAL:C	3:B:177:HOH:O	2.34	0.53
1:B:7:PHE:CE1	1:B:98:LYS:HB2	2.45	0.52
1:A:55:ILE:HD12	1:A:70:THR:HG23	1.92	0.51
1:C:19:LYS:HD2	3:C:118:HOH:O	2.12	0.50
1:B:27:LYS:NZ	3:B:122:HOH:O	2.11	0.47
1:A:61:GLY:CA	3:A:191:HOH:O	2.62	0.47
1:B:29:GLU:CG	3:B:187:HOH:O	2.03	0.46
1:A:60:GLU:OE1	1:A:62:LYS:HE3	2.16	0.45
1:A:55:ILE:CD1	1:A:70:THR:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:NZ	3:C:199:HOH:O	2.48	0.45
1:A:52:GLY:HA2	1:A:74:ALA:HA	1.99	0.44
1:B:60:GLU:HG2	3:B:228:HOH:O	2.20	0.41
1:B:87:ARG:HG3	1:B:103:TYR:CE1	2.56	0.41
1:A:27:LYS:HE2	3:A:145:HOH:O	2.21	0.41
1:C:76:ILE:O	1:C:77:ASN:HB2	2.21	0.41
1:C:52:GLY:HA2	1:C:74:ALA:HA	2.02	0.40

All (17) 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:C:136:HOH:O	3:C:218:HOH:O[3_665]	1.70	0.50
3:B:170:HOH:O	3:B:171:HOH:O[2_664]	1.70	0.50
3:C:182:HOH:O	3:C:183:HOH:O[2_654]	1.73	0.47
3:A:165:HOH:O	3:A:172:HOH:O[3_675]	1.79	0.41
3:A:170:HOH:O	3:B:183:HOH:O[3_564]	1.84	0.36
3:C:207:HOH:O	3:C:208:HOH:O[2_654]	1.88	0.32
3:B:206:HOH:O	3:B:207:HOH:O[2_664]	1.89	0.31
3:A:186:HOH:O	3:A:187:HOH:O[2_764]	1.89	0.31
3:B:221:HOH:O	3:B:222:HOH:O[2_664]	1.97	0.23
3:A:155:HOH:O	3:B:183:HOH:O[2_774]	1.99	0.21
3:C:218:HOH:O	3:C:219:HOH:O[2_654]	1.99	0.21
3:B:186:HOH:O	3:B:216:HOH:O[3_565]	2.08	0.12
3:C:159:HOH:O	3:C:164:HOH:O[2_654]	2.09	0.11
3:B:121:HOH:O	3:C:175:HOH:O[3_675]	2.13	0.07
3:B:178:HOH:O	3:B:179:HOH:O[2_664]	2.13	0.07
3:A:174:HOH:O	3:A:175:HOH:O[2_764]	2.16	0.04
3:B:187:HOH:O	3:C:192:HOH:O[3_675]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	101 (95%)	5 (5%)	0	100	100
1	B	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	C	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
All	All	317/330 (96%)	307 (97%)	10 (3%)	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	88/91 (97%)	87 (99%)	1 (1%)	80	83
1	B	84/91 (92%)	83 (99%)	1 (1%)	78	81
1	C	87/91 (96%)	87 (100%)	0	100	100
All	All	259/273 (95%)	257 (99%)	2 (1%)	86	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LYS
1	B	70	THR

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

Mol	Chain	Res	Type
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.