



wwPDB X-ray Structure Validation Summary Report

Feb 1, 2016 – 11:07 AM GMT

PDB ID : 3O3W
Title : Crystal Structure of BH2092 protein (residues 14-131) from Bacillus halodurans, Northeast Structural Genomics Consortium Target BhR228A
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccocanti, C.; Lee, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-07-26
Resolution : 2.91 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
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

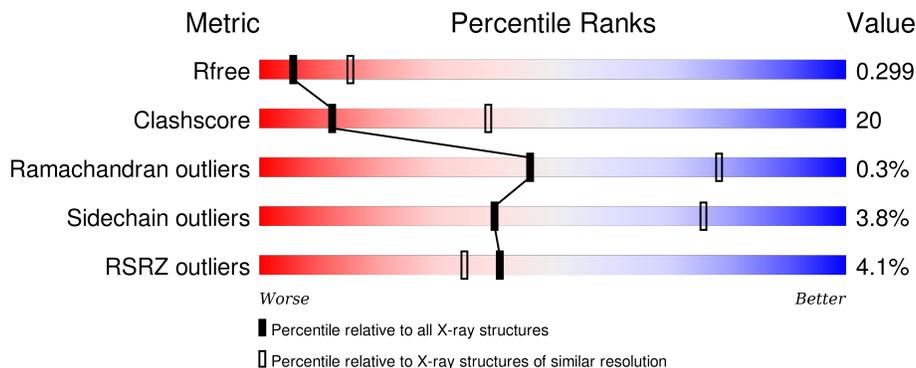
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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))
R_{free}	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	126	
1	B	126	
1	C	126	
1	D	126	
1	E	126	

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Mol	Chain	Length	Quality of chain
1	F	126	
1	G	126	
1	H	126	
1	I	126	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8353 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 BH2092 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	118	928	591	159	174	3	1	0	0	0
1	B	117	928	591	158	175	3	1	0	0	0
1	C	118	933	594	159	176	3	1	0	0	0
1	D	114	907	578	155	170	3	1	0	0	0
1	E	118	933	594	159	176	3	1	0	0	0
1	F	118	929	591	161	173	3	1	0	0	0
1	G	114	907	578	155	170	3	1	0	0	0
1	H	116	919	586	157	172	3	1	0	0	0
1	I	113	890	567	153	166	3	1	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
A	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
A	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
B	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
B	134	HIS	-	EXPRESSION TAG	UNP Q9KB42

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Chain	Residue	Modelled	Actual	Comment	Reference
B	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
C	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
C	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
D	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
D	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
E	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
E	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
F	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
F	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
G	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
G	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	136	HIS	-	EXPRESSION TAG	UNP Q9KB42

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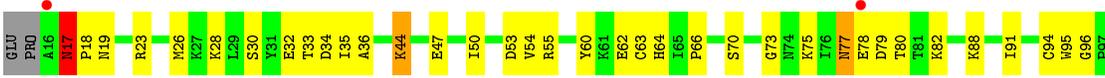
Chain	Residue	Modelled	Actual	Comment	Reference
G	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
H	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
H	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
I	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
I	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	139	HIS	-	EXPRESSION TAG	UNP Q9KB42

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	9	Total O 9 9	0	0
2	C	6	Total O 6 6	0	0
2	D	10	Total O 10 10	0	0
2	E	11	Total O 11 11	0	0
2	F	7	Total O 7 7	0	0
2	G	10	Total O 10 10	0	0
2	H	2	Total O 2 2	0	0
2	I	10	Total O 10 10	0	0

LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: BH2092 protein



• Molecule 1: BH2092 protein



• Molecule 1: BH2092 protein

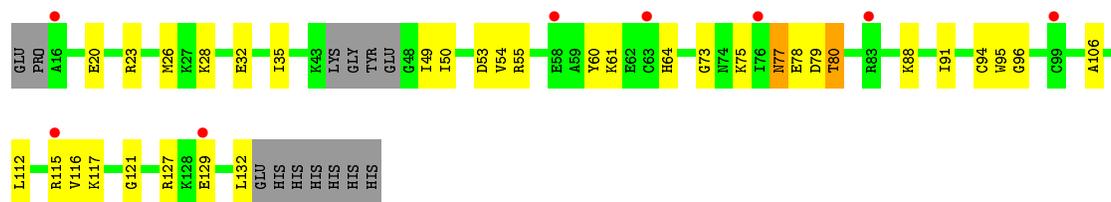


• Molecule 1: BH2092 protein



• Molecule 1: BH2092 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	114.24Å 114.24Å 85.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 2.91 28.56 – 2.91	Depositor EDS
% Data completeness (in resolution range)	93.9 (19.79-2.91) 99.5 (28.56-2.91)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.292 0.261 , 0.299	Depositor DCC
R_{free} test set	2694 reflections (9.91%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 2.1	EDS
Estimated twinning fraction	0.098 for -h,-k,l 0.099 for h,-h-k,-l 0.286 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 54750 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8353	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.48	0/946	0.61	0/1275
1	B	0.45	0/945	0.58	0/1272
1	C	0.49	0/950	1.26	3/1279 (0.2%)
1	D	0.45	0/924	0.57	0/1244
1	E	0.47	0/950	0.60	0/1279
1	F	0.45	0/946	0.59	0/1272
1	G	0.46	0/924	0.55	0/1244
1	H	0.42	0/936	0.55	0/1260
1	I	0.46	0/905	0.56	0/1218
All	All	0.46	0/8426	0.69	3/11343 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	23	ARG	NE-CZ-NH1	-27.41	106.60	120.30
1	C	23	ARG	NE-CZ-NH2	25.63	133.12	120.30
1	C	23	ARG	CD-NE-CZ	12.99	141.78	123.60

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	928	0	927	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	928	0	930	35	0
1	C	933	0	935	56	1
1	D	907	0	910	41	0
1	E	933	0	935	59	0
1	F	929	0	934	47	1
1	G	907	0	910	35	0
1	H	919	0	924	28	0
1	I	890	0	897	41	0
2	A	14	0	0	1	0
2	B	9	0	0	2	0
2	C	6	0	0	1	0
2	D	10	0	0	1	0
2	E	11	0	0	4	0
2	F	7	0	0	2	0
2	G	10	0	0	4	0
2	H	2	0	0	0	0
2	I	10	0	0	6	0
All	All	8353	0	8302	324	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 20.

The worst 5 of 324 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:C:78:GLU:OE1	1:E:26:MSE:HE2	1.37	1.24
1:I:49:ILE:HD12	1:I:91:ILE:HD12	1.37	1.07
1:E:115:ARG:HH12	1:F:15:PRO:HB2	1.17	1.05
1:D:23:ARG:NH2	1:I:20:GLU:HB2	1.73	1.03
1:G:35:ILE:HG21	1:G:129:GLU:HG3	1.42	0.98

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)
1:C:22:TYR:OH	1:F:83:ARG:NH1[2_455]	2.11	0.09

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	116/126 (92%)	108 (93%)	7 (6%)	1 (1%)	21	56
1	B	115/126 (91%)	109 (95%)	6 (5%)	0	100	100
1	C	116/126 (92%)	108 (93%)	7 (6%)	1 (1%)	21	56
1	D	112/126 (89%)	108 (96%)	4 (4%)	0	100	100
1	E	116/126 (92%)	109 (94%)	6 (5%)	1 (1%)	21	56
1	F	114/126 (90%)	106 (93%)	8 (7%)	0	100	100
1	G	112/126 (89%)	103 (92%)	9 (8%)	0	100	100
1	H	114/126 (90%)	105 (92%)	9 (8%)	0	100	100
1	I	109/126 (86%)	102 (94%)	7 (6%)	0	100	100
All	All	1024/1134 (90%)	958 (94%)	63 (6%)	3 (0%)	46	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	ASN
1	A	15	PRO
1	C	132	LEU

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	96/104 (92%)	92 (96%)	4 (4%)	36	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	97/104 (93%)	94 (97%)	3 (3%)	47	81
1	C	97/104 (93%)	93 (96%)	4 (4%)	37	73
1	D	95/104 (91%)	93 (98%)	2 (2%)	61	87
1	E	97/104 (93%)	91 (94%)	6 (6%)	23	54
1	F	97/104 (93%)	91 (94%)	6 (6%)	23	54
1	G	95/104 (91%)	92 (97%)	3 (3%)	46	81
1	H	96/104 (92%)	93 (97%)	3 (3%)	47	81
1	I	93/104 (89%)	91 (98%)	2 (2%)	60	87
All	All	863/936 (92%)	830 (96%)	33 (4%)	40	76

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	44	LYS
1	E	133	GLU
1	H	80	THR
1	E	77	ASN
1	E	80	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	130	ASN
1	E	111	GLN
1	I	77	ASN
1	E	77	ASN
1	F	77	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 [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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	117/126 (92%)	0.20	3 (2%) 59 54	12, 25, 46, 55	0
1	B	116/126 (92%)	0.18	2 (1%) 73 70	6, 25, 47, 52	0
1	C	117/126 (92%)	0.29	2 (1%) 73 70	11, 24, 44, 52	0
1	D	113/126 (89%)	0.19	1 (0%) 85 84	10, 27, 47, 54	0
1	E	117/126 (92%)	0.23	3 (2%) 59 54	5, 23, 46, 55	0
1	F	117/126 (92%)	0.31	2 (1%) 73 70	9, 26, 46, 52	0
1	G	113/126 (89%)	0.73	14 (12%) 5 3	22, 38, 57, 66	0
1	H	115/126 (91%)	0.48	7 (6%) 25 18	24, 37, 55, 69	0
1	I	112/126 (88%)	0.66	8 (7%) 19 13	25, 38, 55, 62	0
All	All	1037/1134 (91%)	0.36	42 (4%) 41 35	5, 31, 51, 69	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	83	ARG	4.3
1	G	115	ARG	4.1
1	G	130	ASN	4.0
1	H	47	GLU	3.5
1	A	131	GLY	3.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.