



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3B55 / pdb_00003b55
Title : Crystal structure of the Q81BN2_BACCR protein from Bacillus cereus.
NESG target BcR135
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Deposited on : 2007-10-25
Resolution : 2.30 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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

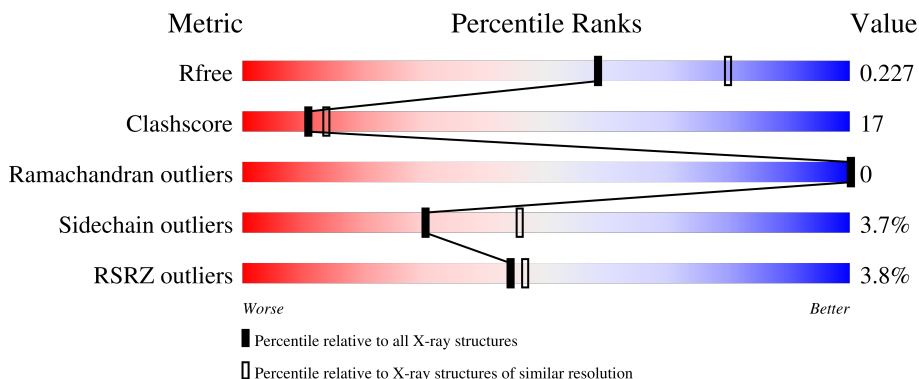
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	451	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3432 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 Succinoglycan biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	Se	0	0	0
			3263	2092	553	610	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	THR	GLN	engineered mutation	UNP Q81BN2
A	444	LEU	-	expression tag	UNP Q81BN2
A	445	GLU	-	expression tag	UNP Q81BN2
A	446	HIS	-	expression tag	UNP Q81BN2
A	447	HIS	-	expression tag	UNP Q81BN2
A	448	HIS	-	expression tag	UNP Q81BN2
A	449	HIS	-	expression tag	UNP Q81BN2
A	450	HIS	-	expression tag	UNP Q81BN2
A	451	HIS	-	expression tag	UNP Q81BN2

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		

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 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.

Chain A:

Item	Category
D381	Green
Q382	Green
F383	Green
F384	Green
K389	Green
A390	Green
N399	Green
A400	Green
Q401	Green
H402	Green
F405	Green
T410	Green
E411	Green
I415	Green
I421	Green
K425	Green
I429	Green
L430	Green
V431	Green
Q432	Green
Q440	Green
V441	Green
H442	Green
Q443	Green
LEU	Green
GLY	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
E289	Orange
K202	Orange
I203	Orange
A290	Green
A291	Green
K292	Green
E295	Green
E296	Green
G299	Green
W304	Green
G305	Green
H306	Green
N307	Green
S311	Green
N314	Green
M315	Green
L316	Orange
I319	Green
Y320	Green
P321	Green
K322	Green
V323	Green
Q326	Green
V337	Green
S338	Green
I339	Green
S342	Green
W343	Green
Y344	Green
E345	Green
N349	Green
V350	Green
K351	Green
E356	Green
F357	Green
G358	Green
P359	Green
Y360	Green
K364	Green
S365	Green
D366	Green
D367	Green
P368	Green
Y371	Green
N372	Green
Y373	Green
V378	Green
H85	Orange
K202	Orange
I203	Orange
K204	Green
I207	Green
K93	Green
K94	Green
H95	Green
R96	Green
I97	Green
V98	Green
K105	Green
T220	Green
K221	Green
E222	Green
E223	Green
K224	Green
V228	Green
L229	Green
T233	Green
A236	Green
L237	Green
E240	Orange
N241	Green
Y244	Green
G247	Green
K248	Green
S249	Green
K250	Green
E251	Green
W254	Green
I255	Green
K256	Green
Q257	Green
N258	Green
A259	Green
R260	Green
Q264	Green
T267	Green
M268	Green
D278	Green
F279	Green
Y280	Green
L281	Green
K282	Green
H283	Green
D284	Green
I285	Orange
A286	Orange
M287	Green
V288	Green
E290	Green
E291	Green
E292	Green
E293	Green
E294	Green
E295	Green
E296	Green
E297	Green
E298	Green
E299	Green
E300	Green
E301	Green
E302	Green
E303	Green
E304	Green
E305	Green
E306	Green
E307	Green
E308	Green
E309	Green
E310	Green
E311	Green
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E313	Green
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E315	Green
E316	Green
E317	Green
E318	Green
E319	Green
E320	Green
E321	Green
E322	Green
E323	Green
E324	Green
E325	Green
E326	Green
E327	Green
E328	Green
E329	Green
E330	Green
E331	Green
E332	Green
E333	Green
E334	Green
E335	Green
E336	Green
E337	Green
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E361	Green
E362	Green
E363	Green
E364	Green
E365	Green
E366	Green
E367	Green
E368	Green
E369	Green
E370	Green
E371	Green
E372	Green
E373	Green
E374	Green
E375	Green
E376	Green
E377	Green
E378	Green
E379	Green
E380	Green

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.89Å 67.71Å 119.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.06 – 2.30 46.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.1 (46.06-2.30) 96.6 (46.06-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.31 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.214 0.204 , 0.227	Depositor DCC
R_{free} test set	1399 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3432	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/3332	0.94	8/4498 (0.2%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	LYS	N-CA-C	-10.80	98.41	111.69
1	A	285	ILE	N-CA-C	-7.36	103.61	110.53
1	A	247	GLY	N-CA-C	6.18	121.33	113.24
1	A	132	ASN	CA-C-N	6.14	127.52	119.84
1	A	132	ASN	C-N-CA	6.14	127.52	119.84

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	3263	0	3261	108	0
2	A	1	0	0	0	0
3	A	168	0	0	6	0
All	All	3432	0	3261	108	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 17.

The worst 5 of 108 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:56:THR:HG22	1:A:93:MSE:HE2	1.29	1.09
1:A:372:ASN:HD21	1:A:405:PHE:H	1.26	0.81
1:A:157:ASN:HD21	1:A:166:VAL:H	1.31	0.79
1:A:144:LYS:HD2	1:A:440:GLN:NE2	1.99	0.76
1:A:220:THR:HG23	1:A:223:GLU:H	1.54	0.72

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	406/451 (90%)	391 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	356/386 (92%)	343 (96%)	13 (4%)	30	45

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	A	240	GLU
1	A	401	GLN
1	A	319	ILE
1	A	322	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	GLN
1	A	399	ASN
1	A	440	GLN
1	A	402	HIS
1	A	391	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](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

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	400/451 (88%)	0.04	15 (3%)	44 46	6, 18, 42, 56	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	TYR	3.6
1	A	201	GLU	3.4
1	A	443	GLN	3.4
1	A	200	GLU	2.9
1	A	411	GLU	2.9

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	CA	A	501	1/1	0.96	0.15	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.