



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 01:02 PM EDT

PDB ID : 2AUA
Title : Structure of BC2332: A Protein of Unknown Function from Bacillus cereus
Authors : Brunzelle, J.S.; Minasov, G.; Shuvalova, L.; Collart, F.R.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2005-08-27
Resolution : 2.35 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

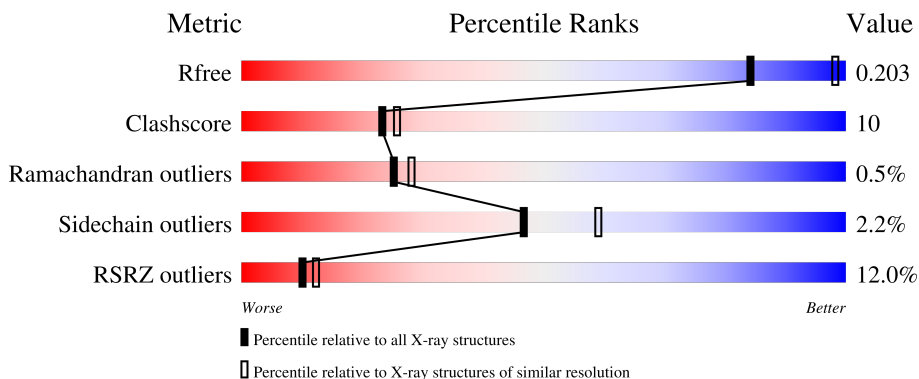
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	224	 6% 74% 13% • 11%
1	B	224	 15% 72% 20% • 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3605 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 hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	199	1691	1079	288	319	1	4	0	8	0
1	B	210	1767	1127	299	335	1	5	0	5	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	cloning artifact	UNP Q81DM5
A	-22	HIS	-	expression tag	UNP Q81DM5
A	-21	HIS	-	expression tag	UNP Q81DM5
A	-20	HIS	-	expression tag	UNP Q81DM5
A	-19	HIS	-	expression tag	UNP Q81DM5
A	-18	HIS	-	expression tag	UNP Q81DM5
A	-17	HIS	-	expression tag	UNP Q81DM5
A	-16	SER	-	cloning artifact	UNP Q81DM5
A	-15	SER	-	cloning artifact	UNP Q81DM5
A	-14	GLY	-	cloning artifact	UNP Q81DM5
A	-13	VAL	-	cloning artifact	UNP Q81DM5
A	-12	ASP	-	cloning artifact	UNP Q81DM5
A	-11	LEU	-	cloning artifact	UNP Q81DM5
A	-10	GLY	-	cloning artifact	UNP Q81DM5
A	-9	THR	-	cloning artifact	UNP Q81DM5
A	-8	GLU	-	cloning artifact	UNP Q81DM5
A	-7	ASN	-	cloning artifact	UNP Q81DM5
A	-6	LEU	-	cloning artifact	UNP Q81DM5
A	-5	TYR	-	cloning artifact	UNP Q81DM5
A	-4	PHE	-	cloning artifact	UNP Q81DM5
A	-3	GLN	-	cloning artifact	UNP Q81DM5
A	-2	SER	-	cloning artifact	UNP Q81DM5
A	-1	ASN	-	cloning artifact	UNP Q81DM5
A	0	ALA	-	cloning artifact	UNP Q81DM5
B	-23	MSE	-	cloning artifact	UNP Q81DM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP Q81DM5
B	-21	HIS	-	expression tag	UNP Q81DM5
B	-20	HIS	-	expression tag	UNP Q81DM5
B	-19	HIS	-	expression tag	UNP Q81DM5
B	-18	HIS	-	expression tag	UNP Q81DM5
B	-17	HIS	-	expression tag	UNP Q81DM5
B	-16	SER	-	cloning artifact	UNP Q81DM5
B	-15	SER	-	cloning artifact	UNP Q81DM5
B	-14	GLY	-	cloning artifact	UNP Q81DM5
B	-13	VAL	-	cloning artifact	UNP Q81DM5
B	-12	ASP	-	cloning artifact	UNP Q81DM5
B	-11	LEU	-	cloning artifact	UNP Q81DM5
B	-10	GLY	-	cloning artifact	UNP Q81DM5
B	-9	THR	-	cloning artifact	UNP Q81DM5
B	-8	GLU	-	cloning artifact	UNP Q81DM5
B	-7	ASN	-	cloning artifact	UNP Q81DM5
B	-6	LEU	-	cloning artifact	UNP Q81DM5
B	-5	TYR	-	cloning artifact	UNP Q81DM5
B	-4	PHE	-	cloning artifact	UNP Q81DM5
B	-3	GLN	-	cloning artifact	UNP Q81DM5
B	-2	SER	-	cloning artifact	UNP Q81DM5
B	-1	ASN	-	cloning artifact	UNP Q81DM5
B	0	ALA	-	cloning artifact	UNP Q81DM5

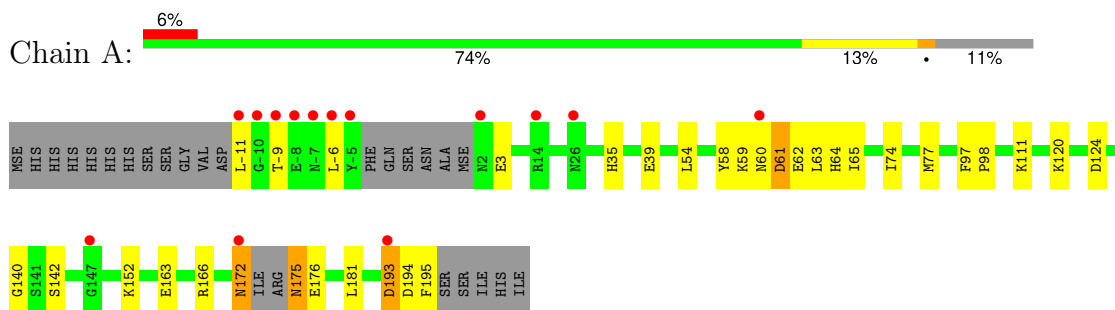
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	62	Total O 63 63	0	1
2	B	84	Total O 84 84	0	0

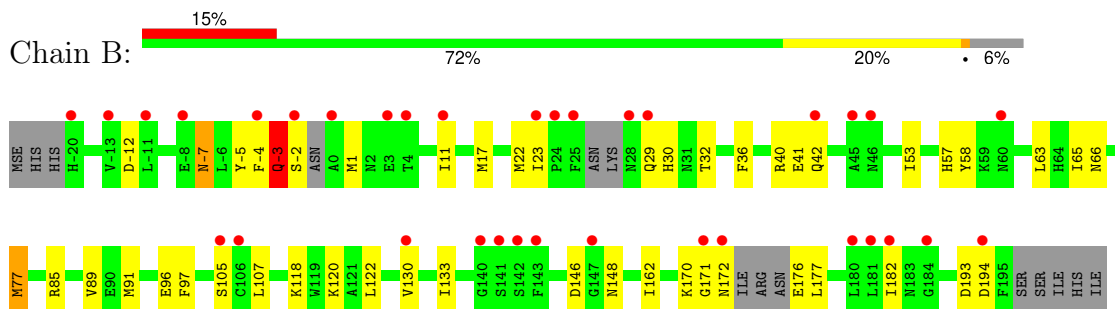
3 Residue-property plots [i](#)

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.

- Molecule 1: hypothetical protein



- Molecule 1: hypothetical protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.22Å 76.64Å 107.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.35) 99.3 (30.00-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.204 , 0.254 0.205 , 0.203	Depositor DCC
R_{free} test set	1262 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3605	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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](#)

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	0.50	0/1748	0.70	4/2350 (0.2%)
1	B	0.52	0/1813	0.71	4/2435 (0.2%)
All	All	0.51	0/3561	0.71	8/4785 (0.2%)

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	1
1	B	0	1
All	All	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($^{\circ}$)	Ideal($^{\circ}$)
1	B	-12	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	61[A]	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	61[B]	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	194	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	193	ASP	CB-CG-OD2	5.37	123.13	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ASN	Peptide
1	B	170	LYS	Peptide

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	1691	0	1654	35	0
1	B	1767	0	1703	50	0
2	A	63	0	0	2	0
2	B	84	0	0	3	0
All	All	3605	0	3357	69	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 10.

The worst 5 of 69 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:17:MSE:HE1	1:B:23:ILE:HD11	1.38	1.05
1:B:176:GLU:CG	1:B:177:LEU:H	1.71	1.03
1:A:77:MSE:HE1	1:B:77:MSE:SE	2.13	0.97
1:B:40:ARG:HG2	1:B:40:ARG:HH11	1.29	0.97
1:B:176:GLU:HG3	1:B:177:LEU:H	1.30	0.95

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	201/224 (90%)	192 (96%)	8 (4%)	1 (0%)	25 28
1	B	207/224 (92%)	199 (96%)	7 (3%)	1 (0%)	25 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	408/448 (91%)	391 (96%)	15 (4%)	2 (0%)	25 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLU
1	B	-3	GLN

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	186/196 (95%)	184 (99%)	2 (1%)	70 81
1	B	193/196 (98%)	187 (97%)	6 (3%)	35 44
All	All	379/392 (97%)	371 (98%)	8 (2%)	47 61

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	MSE
1	B	32	THR
1	B	-2	SER
1	B	-3	GLN
1	B	1	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	-3	GLN
1	B	2	ASN
1	B	66	ASN
1	B	28	ASN
1	A	67	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 [i](#)

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

Warning: The R factor obtained from EDS is 0.2543, which does not match the depositor's R factor of 0.2038. Please interpret the results in this section carefully.

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	195/224 (87%)	0.78	14 (7%) 23 27	26, 48, 68, 85	8 (4%)
1	B	205/224 (91%)	0.98	34 (16%) 5 6	23, 48, 61, 79	5 (2%)
All	All	400/448 (89%)	0.88	48 (12%) 10 12	23, 48, 63, 85	13 (3%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	ASP	6.3
1	B	25	PHE	5.7
1	A	-7	ASN	5.1
1	A	-5	TYR	4.4
1	B	-2	SER	4.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.