



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:02 PM UTC

PDB ID : 3A2N / pdb\_00003a2n  
Title : Crystal structure of DBJA (Wild Type Type II P21)  
Authors : Sato, Y.; Senda, T.  
Deposited on : 2009-05-23  
Resolution : 1.89 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
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

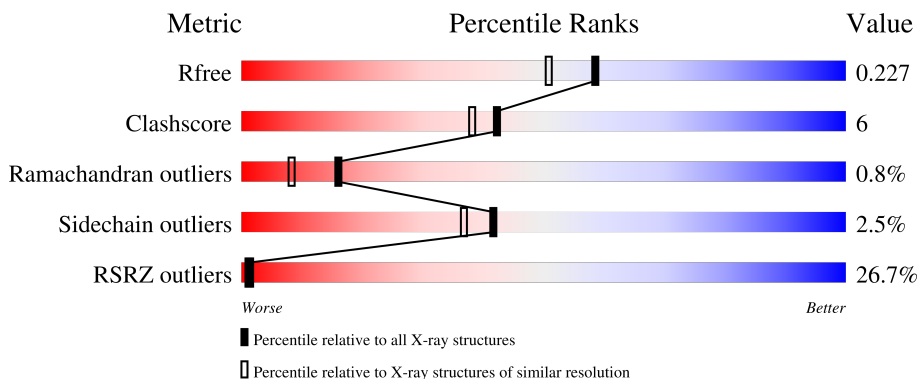
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	312	
1	B	312	
1	E	312	
1	F	312	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9801 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 Haloalkane dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2320	1485	415	413	7	0	0	0
1	B	298	2330	1491	418	414	7	0	1	0
1	E	298	2320	1485	415	413	7	0	0	0
1	F	299	2338	1497	419	415	7	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	VAL	-	SEE REMARK 999	UNP P59337
A	312	ASP	-	SEE REMARK 999	UNP P59337
B	311	VAL	-	SEE REMARK 999	UNP P59337
B	312	ASP	-	SEE REMARK 999	UNP P59337
E	311	VAL	-	SEE REMARK 999	UNP P59337
E	312	ASP	-	SEE REMARK 999	UNP P59337
F	311	VAL	-	SEE REMARK 999	UNP P59337
F	312	ASP	-	SEE REMARK 999	UNP P59337

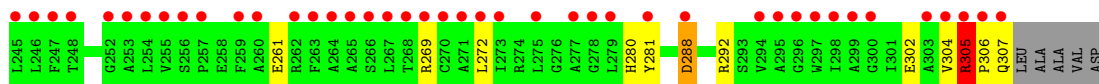
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	B	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

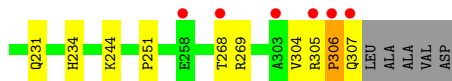
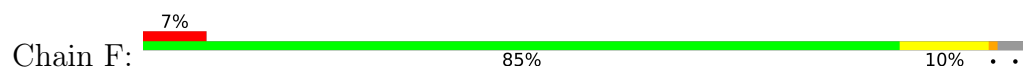
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	0	0
3	B	162	Total 162	O 162	0	0
3	E	45	Total 45	O 45	0	0
3	F	172	Total 173	O 173	0	1





- Molecule 1: Haloalkane dehalogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.53Å 47.77Å 99.41Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	32.81 – 1.89 32.81 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.81-1.89) 99.2 (32.81-1.89)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.17 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.192 , 0.228 0.191 , 0.227	Depositor DCC
$R_{free}$ test set	4719 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtrriage
Anisotropy	0.082	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0884e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL

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	0.73	0/2388	0.83	4/3252 (0.1%)
1	B	0.80	0/2399	0.83	0/3267
1	E	0.94	8/2388 (0.3%)	0.91	2/3252 (0.1%)
1	F	0.82	0/2407	0.88	0/3278
All	All	0.82	8/9582 (0.1%)	0.86	6/13049 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	76	TYR	C-O	17.54	1.46	1.23
1	E	73	ASP	CG-OD2	14.87	1.53	1.25
1	E	73	ASP	CG-OD1	12.32	1.48	1.25
1	E	81	HIS	CE1-NE2	7.66	1.40	1.32
1	E	81	HIS	CG-CD2	6.55	1.43	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	MET	CA-C-N	5.30	125.36	119.32
1	A	132	MET	C-N-CA	5.30	125.36	119.32
1	E	305	ARG	CA-C-N	-5.03	114.77	119.85
1	E	305	ARG	C-N-CA	-5.03	114.77	119.85
1	A	305	ARG	CA-C-N	5.03	126.13	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	2320	0	2268	28	0
1	B	2330	0	2274	33	0
1	E	2320	0	2268	40	0
1	F	2338	0	2285	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
3	A	110	0	0	1	0
3	B	162	0	0	3	0
3	E	45	0	0	3	0
3	F	173	0	0	2	0
All	All	9801	0	9095	115	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 6.

The worst 5 of 115 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:E:188:LYS:HD3	3:E:327:HOH:O	1.57	1.00
1:B:305:ARG:HB2	1:B:306:PRO:HD2	1.44	1.00
1:E:304:VAL:HG21	1:F:304:VAL:HG23	1.63	0.81
1:F:9:ILE:HG23	1:F:21:TYR:O	1.80	0.81
1:B:307:GLN:HG3	1:F:117:PRO:HB3	1.65	0.79

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	296/312 (95%)	282 (95%)	12 (4%)	2 (1%)	18	10
1	B	297/312 (95%)	287 (97%)	8 (3%)	2 (1%)	18	10
1	E	296/312 (95%)	281 (95%)	11 (4%)	4 (1%)	9	3
1	F	298/312 (96%)	289 (97%)	8 (3%)	1 (0%)	36	29
All	All	1187/1248 (95%)	1139 (96%)	39 (3%)	9 (1%)	16	8

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ALA
1	B	305	ARG
1	E	148	ASP
1	E	305	ARG
1	F	306	PRO

### 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	232/244 (95%)	223 (96%)	9 (4%)	28	21
1	B	233/244 (96%)	226 (97%)	7 (3%)	36	30
1	E	232/244 (95%)	229 (99%)	3 (1%)	61	61
1	F	234/244 (96%)	230 (98%)	4 (2%)	53	52
All	All	931/976 (95%)	908 (98%)	23 (2%)	42	37

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	232	SER
1	E	208	ARG
1	E	156	VAL

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Mol	Chain	Res	Type
1	E	288	ASP
1	A	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	234	HIS
1	F	231	GLN
1	F	234	HIS
1	E	81	HIS
1	E	111	HIS

### 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 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/312 (95%)	0.90	32 (10%) 11 11	20, 26, 39, 55	0
1	B	298/312 (95%)	0.52	19 (6%) 25 27	14, 23, 33, 51	1 (0%)
1	E	298/312 (95%)	3.38	246 (82%) 0 0	24, 39, 60, 64	0
1	F	299/312 (95%)	0.53	21 (7%) 22 24	13, 20, 33, 58	1 (0%)
All	All	1193/1248 (95%)	1.34	318 (26%) 1 1	13, 25, 48, 64	2 (0%)

The worst 5 of 318 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	GLN	8.6
1	E	134	THR	7.6
1	B	306	PRO	7.3
1	E	128	PHE	7.2
1	E	132	MET	7.0

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CL	A	313	1/1	0.97	0.10	15,15,15,15	0
2	CL	B	313	1/1	0.99	0.12	12,12,12,12	0
2	CL	F	313	1/1	0.99	0.09	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.