



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:15 AM GMT

PDB ID : 3A2N
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
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

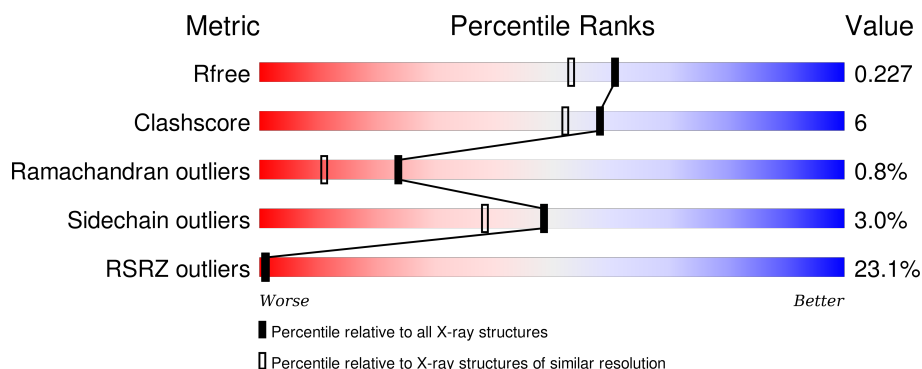
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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	312	<div> <div>18%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	312	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>• •</div> </div> </div>
1	E	312	<div> <div>44%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	F	312	<div> <div>16%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>

2 Entry composition

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
1	A	298	Total	C	N	O	S	0	0	0
			2320	1485	415	413	7			
1	B	298	Total	C	N	O	S	0	1	0
			2330	1491	418	414	7			
1	E	298	Total	C	N	O	S	0	0	0
			2320	1485	415	413	7			
1	F	299	Total	C	N	O	S	0	1	0
			2338	1497	419	415	7			

There are 8 discrepancies between the modelled and reference sequences:

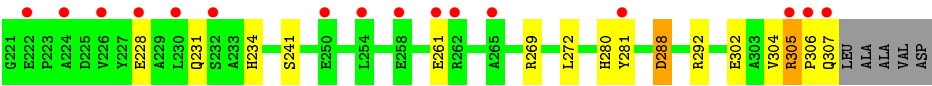
Chain	Residue	Modelled	Actual	Comment	Reference
A	311	VAL	-	SEE REMARK 999	UNP P59337
A	312	ASP	-	SEE REMARK 999	UNP P59337
B	311	VAL	-	SEE REMARK 999	UNP P59337
B	312	ASP	-	SEE REMARK 999	UNP P59337
E	311	VAL	-	SEE REMARK 999	UNP P59337
E	312	ASP	-	SEE REMARK 999	UNP P59337
F	311	VAL	-	SEE REMARK 999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

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

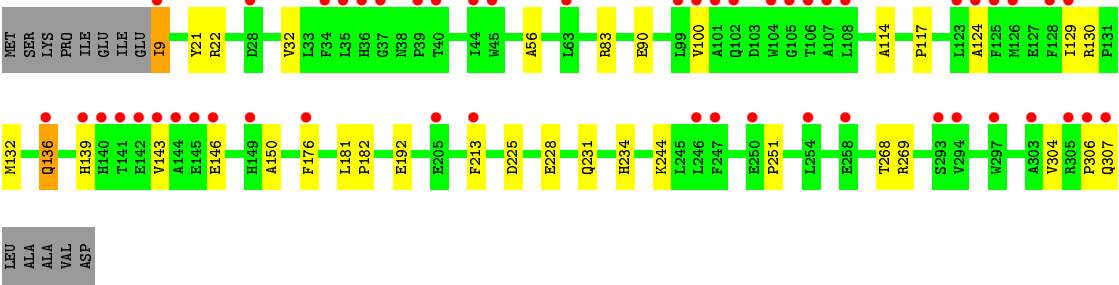
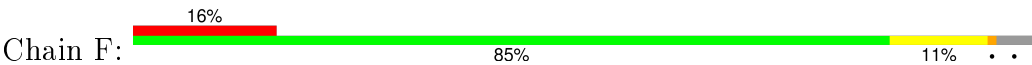
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		

- 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, α , β , γ	125.53 Å 47.77 Å 99.41 Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	32.81 – 1.89 31.49 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.81-1.89) 99.3 (31.49-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.17 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.228 0.191 , 0.227	Depositor DCC
R_{free} test set	4719 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 94027 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9801	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage'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.*

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

5.1 Standard geometry

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	0.59	0/2388	0.61	1/3252 (0.0%)
1	B	0.65	0/2399	0.66	1/3267 (0.0%)
1	E	0.77	6/2388 (0.3%)	0.69	5/3252 (0.2%)
1	F	0.68	0/2407	0.69	2/3278 (0.1%)
All	All	0.68	6/9582 (0.1%)	0.66	9/13049 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	ASP	CG-OD2	12.28	1.53	1.25
1	E	76	TYR	C-O	12.03	1.46	1.23
1	E	73	ASP	CG-OD1	10.18	1.48	1.25
1	E	167	GLU	CD-OE1	8.03	1.34	1.25
1	E	208	ARG	CZ-NH1	6.38	1.41	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	ASP	CB-CG-OD1	-11.52	107.94	118.30
1	E	76	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	E	80	ASP	CB-CG-OD1	7.92	125.42	118.30
1	E	208	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	E	76	TYR	CG-CD2-CE2	-6.24	116.31	121.30

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	32	0
1	E	2320	0	2268	38	0
1	F	2338	0	2285	31	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	109	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 109 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%)	26	14
1	B	297/312 (95%)	287 (97%)	8 (3%)	2 (1%)	26	14
1	E	296/312 (95%)	281 (95%)	11 (4%)	4 (1%)	14	4
1	F	298/312 (96%)	289 (97%)	8 (3%)	1 (0%)	46	35
All	All	1187/1248 (95%)	1139 (96%)	39 (3%)	9 (1%)	24	11

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%)	39	27
1	B	233/244 (96%)	224 (96%)	9 (4%)	39	27
1	E	232/244 (95%)	227 (98%)	5 (2%)	60	53
1	F	234/244 (96%)	229 (98%)	5 (2%)	61	55
All	All	931/976 (95%)	903 (97%)	28 (3%)	48	38

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	156	VAL
1	B	213	PHE
1	F	176	PHE

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Mol	Chain	Res	Type
1	B	176	PHE
1	B	205	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	307	GLN
1	E	111	HIS
1	E	234	HIS
1	B	234	HIS
1	E	231	GLN

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](#)

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, 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	298/312 (95%)	1.11	56 (18%) 2 2	20, 26, 39, 55	0
1	B	298/312 (95%)	0.84	30 (10%) 9 10	18, 23, 33, 51	0
1	E	298/312 (95%)	2.23	138 (46%) 0 0	24, 39, 60, 64	0
1	F	299/312 (95%)	0.96	51 (17%) 2 2	15, 20, 33, 58	0
All	All	1193/1248 (95%)	1.29	275 (23%) 1 1	15, 25, 48, 64	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	GLN	11.5
1	A	306	PRO	10.7
1	B	306	PRO	9.6
1	B	307	GLN	9.4
1	F	307	GLN	9.4

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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CL	F	313	1/1	1.00	0.06	-3.74	10,10,10,10	0
2	CL	A	313	1/1	0.99	0.04	-4.37	15,15,15,15	0
2	CL	B	313	1/1	0.99	0.05	-4.70	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.