



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:21 PM UTC

PDB ID : 4OFW / pdb_00004ofw
Title : Crystal Structure of Arabidopsis thaliana DJ-1d
Authors : Choi, D.; Kim, J.; Ryu, K.-S.; Park, C.
Deposited on : 2014-01-15
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
Xtrriage (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

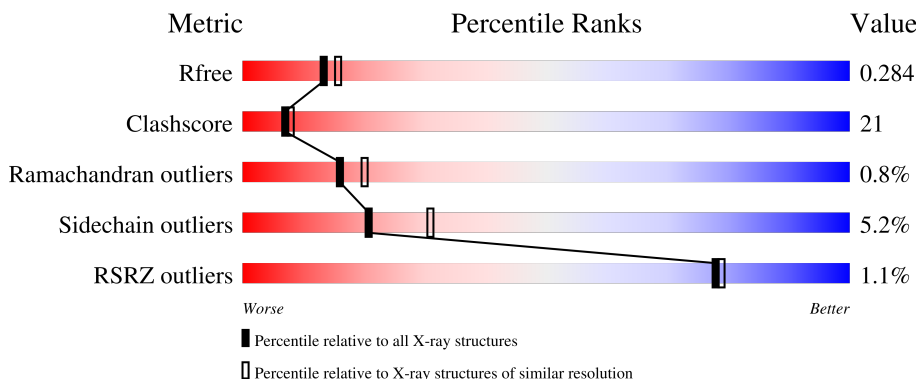
1 Overall quality at a glance

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	387	
1	B	387	
1	C	387	
1	D	387	
1	E	387	

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Mol	Chain	Length	Quality of chain
1	F	387	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '61%', a large yellow segment labeled '35%', and a very small orange segment at the end. A small black dot is visible at the far right end of the bar.</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18086 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 Protein DJ-1 homolog D.

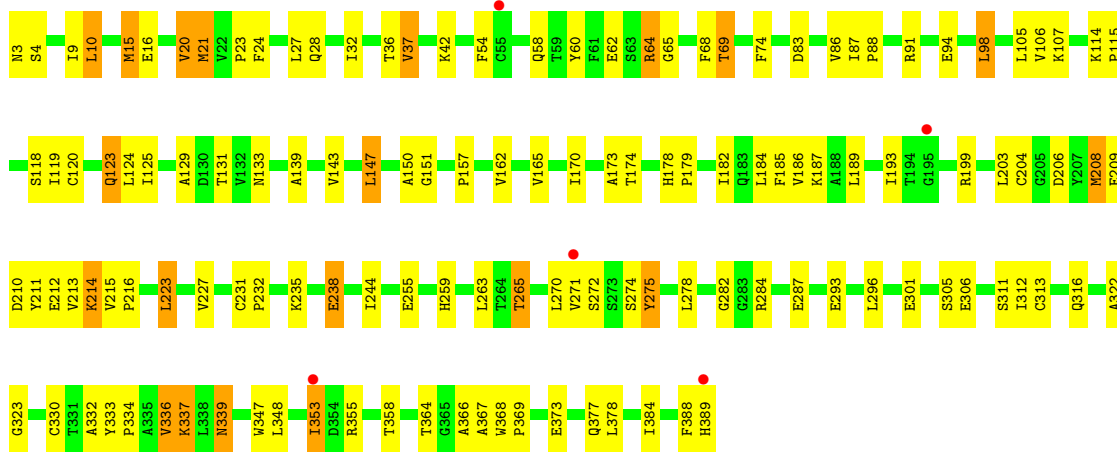
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	2924	1864	487	554	19	0	0	0
1	B	387	2924	1864	487	554	19	0	0	0
1	C	387	2924	1864	487	554	19	0	0	0
1	D	387	2924	1864	487	554	19	0	0	0
1	E	387	2924	1864	487	554	19	0	0	0
1	F	387	2924	1864	487	554	19	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

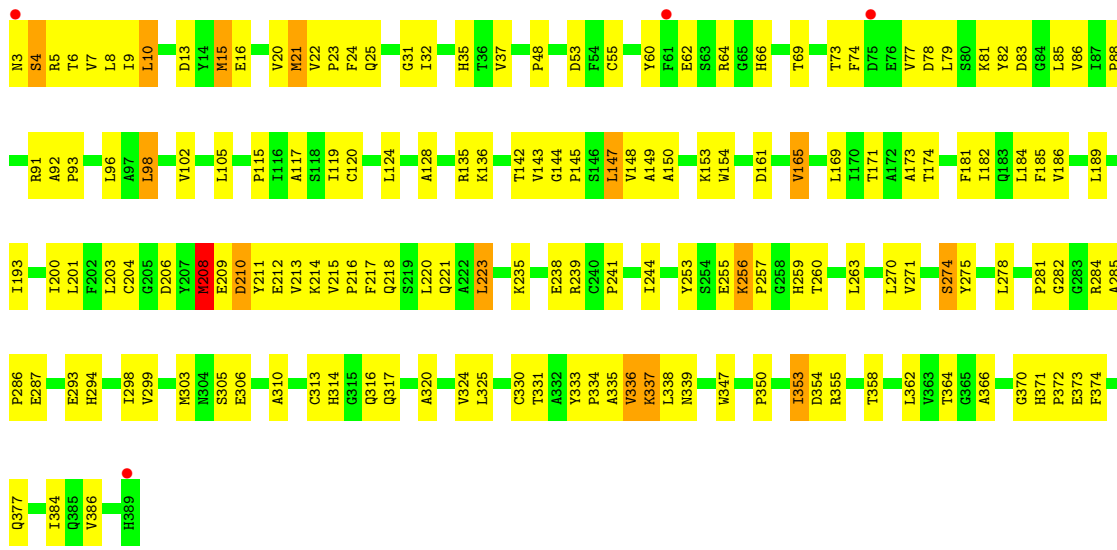
Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	ASP	conflict	UNP Q9M8R4
A	389	HIS	-	expression tag	UNP Q9M8R4
B	238	GLU	ASP	conflict	UNP Q9M8R4
B	389	HIS	-	expression tag	UNP Q9M8R4
C	238	GLU	ASP	conflict	UNP Q9M8R4
C	389	HIS	-	expression tag	UNP Q9M8R4
D	238	GLU	ASP	conflict	UNP Q9M8R4
D	389	HIS	-	expression tag	UNP Q9M8R4
E	238	GLU	ASP	conflict	UNP Q9M8R4
E	389	HIS	-	expression tag	UNP Q9M8R4
F	238	GLU	ASP	conflict	UNP Q9M8R4
F	389	HIS	-	expression tag	UNP Q9M8R4

- Molecule 2 is water.

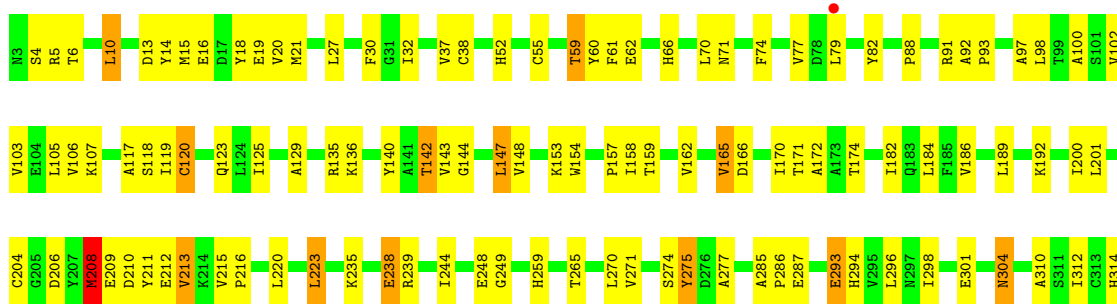
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	97	Total O 97 97	0	0
2	B	81	Total O 81 81	0	0
2	C	96	Total O 96 96	0	0
2	D	100	Total O 100 100	0	0
2	E	82	Total O 82 82	0	0
2	F	86	Total O 86 86	0	0



• Molecule 1: Protein DJ-1 homolog D

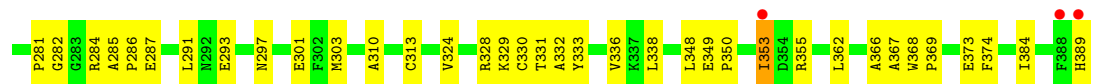
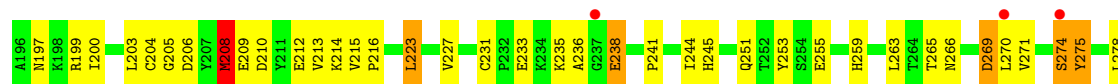
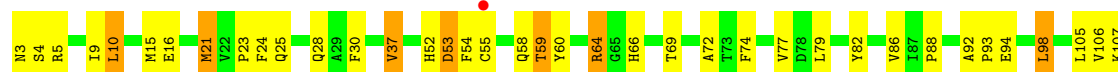


• Molecule 1: Protein DJ-1 homolog D





● Molecule 1: Protein DJ-1 homolog D



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 115.05Å 115.53Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.30) 95.8 (50.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.29Å)	Xtrriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.243 , 0.284 0.243 , 0.284	Depositor DCC
R_{free} test set	11742 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtrriage
Anisotropy	0.678	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.029 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18086	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 46.23 % 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 1.1795e-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, 0.333 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	0.45	0/2994	0.94	8/4075 (0.2%)
1	B	0.43	0/2994	0.96	5/4075 (0.1%)
1	C	0.46	0/2994	0.96	12/4075 (0.3%)
1	D	0.44	0/2994	0.95	11/4075 (0.3%)
1	E	0.43	0/2994	0.93	2/4075 (0.0%)
1	F	0.46	1/2994 (0.0%)	0.94	5/4075 (0.1%)
All	All	0.44	1/17964 (0.0%)	0.95	43/24450 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	21	MET	SD-CE	-5.31	1.66	1.79

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	LYS	N-CA-C	-7.08	103.61	111.82
1	A	208	MET	N-CA-C	-6.77	101.60	110.53
1	F	208	MET	N-CA-C	-6.74	100.51	110.48
1	B	208	MET	N-CA-C	-6.72	101.65	110.53
1	F	227	VAL	N-CA-C	6.72	117.97	108.36

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	2924	0	2872	136	0
1	B	2924	0	2872	124	0
1	C	2924	0	2872	114	0
1	D	2924	0	2872	127	0
1	E	2924	0	2872	120	0
1	F	2924	0	2872	139	0
2	A	97	0	0	23	0
2	B	81	0	0	11	0
2	C	96	0	0	14	0
2	D	100	0	0	20	0
2	E	82	0	0	13	0
2	F	86	0	0	15	0
All	All	18086	0	17232	729	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 21.

The worst 5 of 729 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:F:21:MET:HE2	1:F:25:GLN:HG3	1.35	1.06
1:B:197:ASN:HA	2:B:468:HOH:O	1.59	1.00
1:F:133:ASN:HA	2:F:460:HOH:O	1.66	0.95
1:B:20:VAL:HB	2:B:455:HOH:O	1.66	0.94
1:F:353:ILE:HD12	1:F:353:ILE:H	1.28	0.94

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	385/387 (100%)	353 (92%)	27 (7%)	5 (1%)	9 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	385/387 (100%)	356 (92%)	27 (7%)	2 (0%)	24	31
1	C	385/387 (100%)	356 (92%)	28 (7%)	1 (0%)	36	46
1	D	385/387 (100%)	358 (93%)	24 (6%)	3 (1%)	16	20
1	E	385/387 (100%)	352 (91%)	31 (8%)	2 (0%)	24	31
1	F	385/387 (100%)	356 (92%)	24 (6%)	5 (1%)	9	10
All	All	2310/2322 (100%)	2131 (92%)	161 (7%)	18 (1%)	16	20

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	E	238	GLU
1	A	74	PHE
1	A	236	ALA
1	D	275	TYR

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	313/313 (100%)	292 (93%)	21 (7%)	15	21
1	B	313/313 (100%)	300 (96%)	13 (4%)	26	40
1	C	313/313 (100%)	295 (94%)	18 (6%)	18	26
1	D	313/313 (100%)	297 (95%)	16 (5%)	21	32
1	E	313/313 (100%)	299 (96%)	14 (4%)	24	37
1	F	313/313 (100%)	298 (95%)	15 (5%)	23	35
All	All	1878/1878 (100%)	1781 (95%)	97 (5%)	21	31

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	147	LEU

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Mol	Chain	Res	Type
1	E	142	THR
1	D	208	MET
1	D	336	VAL
1	E	208	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	133	ASN
1	F	221	GLN
1	C	226	GLN
1	C	133	ASN
1	F	259	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](#)

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	387/387 (100%)	0.12	3 (0%) 82 83	16, 30, 48, 69	0
1	B	387/387 (100%)	0.20	2 (0%) 87 87	14, 33, 49, 68	0
1	C	387/387 (100%)	0.06	5 (1%) 75 76	15, 28, 46, 68	0
1	D	387/387 (100%)	0.14	4 (1%) 79 80	18, 31, 49, 69	0
1	E	387/387 (100%)	0.07	3 (0%) 82 83	15, 31, 47, 68	0
1	F	387/387 (100%)	0.16	9 (2%) 61 63	14, 31, 48, 67	0
All	All	2322/2322 (100%)	0.12	26 (1%) 78 79	14, 31, 48, 69	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASN	3.4
1	E	350	PRO	3.3
1	A	389	HIS	3.2
1	F	353	ILE	3.0
1	B	389	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.