



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:47 PM UTC

PDB ID : 5L25 / pdb_00005l25
Title : Crystal Structure of Arabidopsis thaliana Bor1
Authors : Thurtle-Schmidt, B.H.; Stroud, R.M.
Deposited on : 2016-07-31
Resolution : 4.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

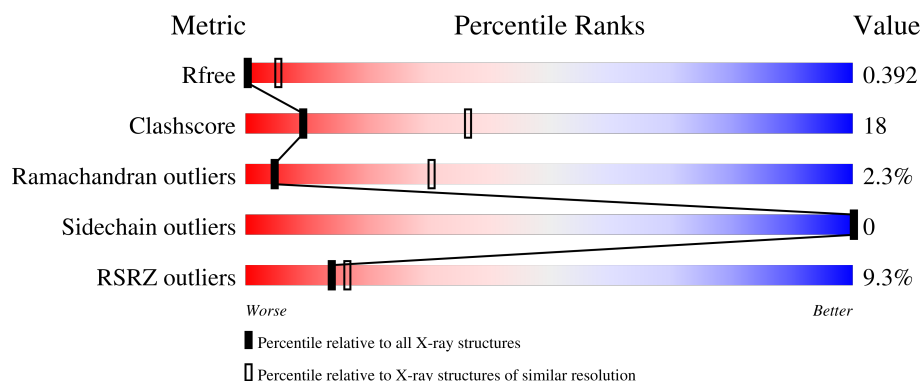
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.11 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	1249 (4.44-3.80)
Clashscore	190562	1031 (4.42-3.82)
Ramachandran outliers	187476	1211 (4.44-3.80)
Sidechain outliers	187428	1198 (4.44-3.80)
RSRZ outliers	180081	1246 (4.44-3.80)

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	652	6% 43% 17% 39%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2873 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 Boron transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			2873	1897	461	495	20			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	646	ALA	-	expression tag	UNP Q8VYR7
A	647	ALA	-	expression tag	UNP Q8VYR7
A	648	ALA	-	expression tag	UNP Q8VYR7
A	649	LEU	-	expression tag	UNP Q8VYR7
A	650	VAL	-	expression tag	UNP Q8VYR7
A	651	PRO	-	expression tag	UNP Q8VYR7
A	652	ARG	-	expression tag	UNP Q8VYR7

- Molecule 1: Boron transporter 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	184.56Å 184.56Å 89.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.07 – 4.11 20.07 – 4.11	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.07-4.11) 94.8 (20.07-4.11)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.359 , 0.391 0.360 , 0.392	Depositor DCC
R_{free} test set	565 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	223.8	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 180.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2873	wwPDB-VP
Average B, all atoms (Å ²)	258.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.69	0/2935	0.86	11/4005 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	PHE	N-CA-C	12.44	124.38	111.07
1	A	155	ALA	N-CA-C	11.69	124.03	111.28
1	A	194	PRO	N-CA-CB	9.51	113.23	103.25
1	A	149	ASN	N-CA-C	8.38	120.03	111.07
1	A	539	PRO	N-CA-CB	7.57	111.05	103.48
1	A	254	PRO	N-CA-CB	6.69	110.36	103.00
1	A	182	PRO	N-CA-CB	6.62	110.20	103.25
1	A	573	MET	N-CA-C	-6.11	104.53	111.07
1	A	482	PRO	N-CA-CB	5.82	109.36	103.25
1	A	153	ARG	N-CA-C	5.60	117.39	111.28
1	A	35	ARG	N-CA-C	5.20	116.63	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2873	0	2721	100	0
All	All	2873	0	2721	100	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 18.

All (100) 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:553:TYR:CE1	1:A:577:LEU:HD12	1.46	1.50
1:A:553:TYR:OH	1:A:574:ILE:N	1.62	1.32
1:A:553:TYR:OH	1:A:573:MET:C	1.91	1.13
1:A:553:TYR:CD1	1:A:577:LEU:CD1	2.35	1.09
1:A:553:TYR:CD1	1:A:577:LEU:HD12	1.88	1.09
1:A:553:TYR:CE1	1:A:577:LEU:CD1	2.36	1.08
1:A:553:TYR:CD1	1:A:577:LEU:HD13	2.08	0.89
1:A:546:PHE:CD1	1:A:549:PHE:HD1	1.90	0.89
1:A:553:TYR:OH	1:A:574:ILE:CA	2.20	0.89
1:A:546:PHE:CD1	1:A:549:PHE:CD1	2.64	0.86
1:A:553:TYR:HE1	1:A:577:LEU:HD12	1.05	0.85
1:A:169:GLN:O	1:A:172:ILE:HG12	1.78	0.83
1:A:480:ALA:O	1:A:484:LEU:CB	2.26	0.83
1:A:553:TYR:HD1	1:A:577:LEU:CD1	1.92	0.82
1:A:546:PHE:O	1:A:548:LEU:N	2.15	0.79
1:A:553:TYR:HD1	1:A:577:LEU:HD13	1.46	0.78
1:A:93:LEU:HD23	1:A:94:GLY:N	2.01	0.75
1:A:54:PHE:HB3	1:A:100:VAL:HG21	1.69	0.75
1:A:553:TYR:HH	1:A:574:ILE:N	1.81	0.74
1:A:34:PHE:HA	1:A:37:LEU:HD12	1.73	0.70
1:A:78:CYS:C	1:A:93:LEU:HD11	2.16	0.70
1:A:553:TYR:OH	1:A:574:ILE:HA	1.90	0.70
1:A:91:LEU:O	1:A:93:LEU:N	2.25	0.70
1:A:169:GLN:O	1:A:172:ILE:CG1	2.40	0.69
1:A:546:PHE:O	1:A:547:THR:C	2.36	0.68
1:A:574:ILE:HG23	1:A:578:ILE:HD12	1.75	0.67
1:A:201:GLY:O	1:A:205:LEU:HB2	1.97	0.65
1:A:56:GLU:HA	1:A:59:GLU:HB2	1.78	0.65
1:A:291:ILE:O	1:A:294:ILE:HG22	1.97	0.64
1:A:57:GLN:HE21	1:A:496:PHE:HE1	1.47	0.63
1:A:560:LEU:HB3	1:A:566:ALA:HB1	1.78	0.63
1:A:552:THR:O	1:A:556:ILE:HG13	1.98	0.63
1:A:577:LEU:O	1:A:581:ARG:HG3	1.98	0.62
1:A:553:TYR:CE2	1:A:578:ILE:HD11	2.36	0.61
1:A:163:ILE:O	1:A:167:PHE:HB2	2.01	0.60
1:A:174:GLY:HA3	1:A:493:TRP:CD2	2.36	0.60
1:A:357:VAL:HG12	1:A:359:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:CYS:HA	1:A:480:ALA:HB3	1.84	0.60
1:A:58:LEU:HD22	1:A:66:LEU:HD23	1.86	0.58
1:A:79:GLY:HA2	1:A:93:LEU:HD13	1.86	0.57
1:A:158:LEU:HD23	1:A:553:TYR:HD2	1.70	0.57
1:A:241:PRO:O	1:A:244:VAL:HB	2.04	0.57
1:A:200:ASN:HA	1:A:203:PHE:HB2	1.87	0.56
1:A:546:PHE:C	1:A:548:LEU:N	2.60	0.56
1:A:93:LEU:HD23	1:A:93:LEU:C	2.31	0.55
1:A:553:TYR:HE1	1:A:577:LEU:CD1	1.96	0.55
1:A:546:PHE:CZ	1:A:549:PHE:HB2	2.42	0.55
1:A:546:PHE:CE1	1:A:549:PHE:HB2	2.42	0.55
1:A:78:CYS:CB	1:A:93:LEU:HD11	2.39	0.52
1:A:137:PHE:CD2	1:A:337:LEU:HD11	2.44	0.52
1:A:337:LEU:O	1:A:339:LEU:N	2.43	0.52
1:A:569:MET:O	1:A:573:MET:HG2	2.10	0.50
1:A:79:GLY:N	1:A:93:LEU:HD11	2.28	0.49
1:A:79:GLY:CA	1:A:93:LEU:HD13	2.43	0.49
1:A:78:CYS:HB2	1:A:93:LEU:HD11	1.93	0.48
1:A:195:SER:HA	1:A:199:ALA:HB3	1.96	0.48
1:A:581:ARG:O	1:A:585:LEU:HG	2.13	0.48
1:A:174:GLY:HA3	1:A:493:TRP:CE3	2.49	0.48
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.96	0.48
1:A:495:TYR:O	1:A:496:PHE:C	2.57	0.47
1:A:123:ALA:O	1:A:126:GLY:N	2.48	0.47
1:A:504:LEU:HB2	1:A:505:PRO:HD3	1.97	0.47
1:A:546:PHE:CE1	1:A:549:PHE:CD1	3.03	0.47
1:A:221:ALA:HB3	1:A:236:ALA:HB2	1.97	0.46
1:A:169:GLN:HA	1:A:172:ILE:HG12	1.98	0.46
1:A:172:ILE:HG13	1:A:173:LYS:N	2.30	0.46
1:A:510:TRP:O	1:A:513:ILE:HG22	2.16	0.46
1:A:492:LEU:O	1:A:496:PHE:HD2	1.99	0.45
1:A:546:PHE:O	1:A:549:PHE:N	2.34	0.45
1:A:203:PHE:O	1:A:490:SER:OG	2.22	0.45
1:A:55:GLY:HA2	1:A:71:THR:OG1	2.17	0.45
1:A:211:LEU:HD21	1:A:495:TYR:CD1	2.52	0.44
1:A:492:LEU:HA	1:A:495:TYR:HD2	1.81	0.44
1:A:491:VAL:HG12	1:A:495:TYR:CE2	2.52	0.44
1:A:495:TYR:HB3	1:A:499:MET:HE2	2.00	0.44
1:A:492:LEU:O	1:A:495:TYR:HB2	2.17	0.44
1:A:79:GLY:N	1:A:93:LEU:CD1	2.81	0.43
1:A:557:CYS:O	1:A:561:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:C	1:A:93:LEU:CD2	2.92	0.43
1:A:308:TYR:CE1	1:A:355:ASN:HB3	2.54	0.43
1:A:58:LEU:HD21	1:A:100:VAL:HG13	2.01	0.43
1:A:233:SER:HA	1:A:236:ALA:HB3	2.01	0.43
1:A:304:ILE:HG23	1:A:308:TYR:CD2	2.54	0.43
1:A:307:LEU:HD12	1:A:571:PRO:HG3	2.01	0.43
1:A:50:PRO:HA	1:A:53:SER:HB3	2.01	0.43
1:A:139:LEU:HB2	1:A:309:TYR:OH	2.19	0.42
1:A:78:CYS:C	1:A:93:LEU:CD1	2.90	0.42
1:A:304:ILE:HG23	1:A:308:TYR:CE2	2.54	0.42
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.86	0.42
1:A:127:TRP:HB3	1:A:294:ILE:HD11	2.02	0.42
1:A:169:GLN:C	1:A:172:ILE:HG12	2.42	0.42
1:A:211:LEU:HD23	1:A:494:GLY:C	2.44	0.42
1:A:514:LEU:HD23	1:A:514:LEU:HA	1.88	0.42
1:A:495:TYR:O	1:A:498:PHE:N	2.53	0.41
1:A:466:SER:HA	1:A:469:LEU:HD12	2.01	0.41
1:A:206:VAL:HA	1:A:209:PHE:CZ	2.56	0.41
1:A:300:PRO:O	1:A:304:ILE:HB	2.21	0.41
1:A:209:PHE:CD1	1:A:210:GLY:N	2.89	0.40
1:A:339:LEU:O	1:A:343:THR:HG23	2.21	0.40
1:A:224:TRP:O	1:A:232:ARG:NH1	2.54	0.40

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	383/652 (59%)	334 (87%)	40 (10%)	9 (2%)	5	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ILE
1	A	203	PHE
1	A	338	LEU
1	A	535	VAL
1	A	82	HIS
1	A	117	GLY
1	A	369	ALA
1	A	193	LEU
1	A	194	PRO

5.3.2 Protein sidechains ⓘ

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	265/553 (48%)	265 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	A	550	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	399/652 (61%)	0.46	37 (9%) 14 17	129, 249, 382, 500	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	PHE	7.8
1	A	363	MET	7.4
1	A	69	VAL	5.1
1	A	159	PHE	5.1
1	A	489	THR	4.9
1	A	523	ARG	4.8
1	A	160	GLY	4.7
1	A	229	GLY	3.9
1	A	146	SER	3.9
1	A	156	GLY	3.8
1	A	141	ILE	3.7
1	A	203	PHE	3.6
1	A	122	LEU	3.6
1	A	359	PRO	3.3
1	A	323	GLU	2.9
1	A	45	PHE	2.9
1	A	142	CYS	2.9
1	A	157	GLU	2.9
1	A	522	ARG	2.8
1	A	108	ASN	2.6
1	A	562	TRP	2.5
1	A	177	ASP	2.5
1	A	152	THR	2.5
1	A	346	CYS	2.4
1	A	520	PRO	2.4
1	A	556	ILE	2.4
1	A	120	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	472	THR	2.3
1	A	70	GLN	2.3
1	A	176	VAL	2.3
1	A	228	THR	2.2
1	A	506	GLY	2.2
1	A	519	ALA	2.2
1	A	369	ALA	2.1
1	A	137	PHE	2.0
1	A	197	ARG	2.0
1	A	204	ALA	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.