



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 02:28 PM JST

PDB ID : 6JEL
Title : Structure of Phytolacca americana apo UGT2
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Deposited on : 2019-02-06
Resolution : 2.30 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

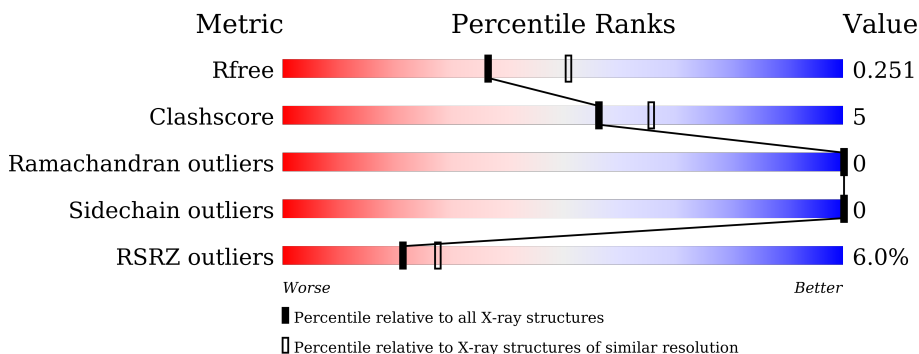
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	489	
1	B	489	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7120 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3499	2242	593	652	12	0	0	0
1	B	451	3472	2227	588	645	12	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B5MGN7
A	-18	ASN	-	expression tag	UNP B5MGN7
A	-17	HIS	-	expression tag	UNP B5MGN7
A	-16	LYS	-	expression tag	UNP B5MGN7
A	-15	VAL	-	expression tag	UNP B5MGN7
A	-14	HIS	-	expression tag	UNP B5MGN7
A	-13	HIS	-	expression tag	UNP B5MGN7
A	-12	HIS	-	expression tag	UNP B5MGN7
A	-11	HIS	-	expression tag	UNP B5MGN7
A	-10	HIS	-	expression tag	UNP B5MGN7
A	-9	HIS	-	expression tag	UNP B5MGN7
A	-8	LEU	-	expression tag	UNP B5MGN7
A	-7	GLN	-	expression tag	UNP B5MGN7
A	-6	GLU	-	expression tag	UNP B5MGN7
A	-5	ASN	-	expression tag	UNP B5MGN7
A	-4	LEU	-	expression tag	UNP B5MGN7
A	-3	TYR	-	expression tag	UNP B5MGN7
A	-2	PHE	-	expression tag	UNP B5MGN7
A	-1	GLN	-	expression tag	UNP B5MGN7
A	0	GLY	-	expression tag	UNP B5MGN7
A	211	ASN	TYR	See sequence details	UNP B5MGN7
B	-19	MET	-	initiating methionine	UNP B5MGN7
B	-18	ASN	-	expression tag	UNP B5MGN7
B	-17	HIS	-	expression tag	UNP B5MGN7
B	-16	LYS	-	expression tag	UNP B5MGN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	VAL	-	expression tag	UNP B5MGN7
B	-14	HIS	-	expression tag	UNP B5MGN7
B	-13	HIS	-	expression tag	UNP B5MGN7
B	-12	HIS	-	expression tag	UNP B5MGN7
B	-11	HIS	-	expression tag	UNP B5MGN7
B	-10	HIS	-	expression tag	UNP B5MGN7
B	-9	HIS	-	expression tag	UNP B5MGN7
B	-8	LEU	-	expression tag	UNP B5MGN7
B	-7	GLN	-	expression tag	UNP B5MGN7
B	-6	GLU	-	expression tag	UNP B5MGN7
B	-5	ASN	-	expression tag	UNP B5MGN7
B	-4	LEU	-	expression tag	UNP B5MGN7
B	-3	TYR	-	expression tag	UNP B5MGN7
B	-2	PHE	-	expression tag	UNP B5MGN7
B	-1	GLN	-	expression tag	UNP B5MGN7
B	0	GLY	-	expression tag	UNP B5MGN7
B	211	ASN	TYR	See sequence details	UNP B5MGN7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	81	Total O 81 81	0	0
2	B	68	Total O 68 68	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.69Å 94.82Å 115.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.64 – 2.30 36.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.64-2.30) 99.9 (36.61-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.220 , 0.251 0.220 , 0.251	Depositor DCC
R_{free} test set	2231 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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	0.40	0/3587	0.58	0/4892
1	B	0.35	0/3559	0.58	0/4852
All	All	0.37	0/7146	0.58	0/9744

There are no bond length outliers.

There are no bond angle outliers.

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	3499	0	3499	33	0
1	B	3472	0	3473	42	0
2	A	81	0	0	3	0
2	B	68	0	0	3	0
All	All	7120	0	6972	70	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 5.

All (70) 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:279:ASN:OD1	1:A:303:PRO:HG3	1.48	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:SER:HA	1:B:301:ARG:NH2	1.72	1.03
1:A:13:SER:N	1:A:115:ASP:OD2	1.93	0.99
1:B:13:SER:N	1:B:115:ASP:OD2	1.95	0.99
1:B:273:SER:HA	1:B:301:ARG:HH21	1.34	0.91
1:A:273:SER:HA	1:A:301:ARG:HH11	1.43	0.80
1:A:253:ASP:HA	1:A:256:LYS:HD2	1.65	0.77
1:B:48:THR:HG23	1:B:51:GLN:H	1.50	0.77
1:A:81:HIS:NE2	1:B:306:HIS:HB3	2.05	0.71
1:B:347:ILE:HG13	2:B:538:HOH:O	1.88	0.71
1:A:49:LYS:HE2	1:A:53:THR:HG21	1.73	0.71
1:A:361:HIS:HD2	1:A:363:GLY:H	1.39	0.70
1:B:48:THR:HG22	1:B:51:GLN:HG3	1.74	0.67
1:A:280:GLU:OE2	1:A:408:ARG:NH2	2.29	0.66
1:A:115:ASP:OD1	2:A:501:HOH:O	2.14	0.65
1:B:48:THR:HG22	1:B:51:GLN:CG	2.27	0.63
1:A:460:VAL:O	1:A:463:LYS:HG2	2.02	0.58
1:B:254:CYS:HB2	1:B:297:LEU:HD11	1.85	0.58
1:A:126:ARG:HH11	1:A:126:ARG:HG3	1.69	0.57
1:B:48:THR:CG2	1:B:51:GLN:H	2.18	0.55
1:A:115:ASP:CG	2:A:501:HOH:O	2.43	0.55
1:A:81:HIS:NE2	1:B:306:HIS:CB	2.70	0.55
1:B:44:THR:HG22	1:B:70:VAL:CG2	2.37	0.55
1:B:284:GLU:HG3	1:B:410:LEU:HD11	1.89	0.55
1:B:273:SER:HA	1:B:301:ARG:HH22	1.70	0.53
1:B:115:ASP:CG	2:B:501:HOH:O	2.47	0.53
1:A:361:HIS:CD2	1:A:363:GLY:H	2.22	0.52
1:B:160:TYR:O	1:B:177:GLY:HA3	2.08	0.52
1:A:160:TYR:O	1:A:177:GLY:HA3	2.09	0.52
1:A:254:CYS:HB2	1:A:297:LEU:HD11	1.91	0.52
1:A:385:GLU:HB2	1:A:388:MET:HE2	1.91	0.52
1:B:273:SER:CA	1:B:301:ARG:NH2	2.61	0.51
1:A:379:VAL:HG13	1:A:400:ALA:HB1	1.94	0.50
1:B:44:THR:HG22	1:B:70:VAL:HG22	1.94	0.50
1:A:385:GLU:HB2	1:A:388:MET:CE	2.42	0.50
1:B:285:LEU:HA	1:B:416:ILE:HD13	1.95	0.49
1:B:48:THR:CG2	1:B:51:GLN:HG3	2.40	0.49
1:B:298:TRP:CE2	1:B:300:VAL:HG12	2.48	0.49
1:A:272:GLY:HA3	1:A:361:HIS:HE1	1.79	0.48
1:B:379:VAL:HG13	1:B:400:ALA:HB1	1.96	0.48
1:A:272:GLY:N	1:A:361:HIS:CE1	2.83	0.47
1:A:13:SER:CB	1:A:115:ASP:OD2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:GLU:HB2	1:B:388:MET:HE2	1.98	0.46
1:A:273:SER:HA	1:A:301:ARG:NH1	2.23	0.46
1:B:115:ASP:OD1	2:B:501:HOH:O	2.21	0.45
1:B:24:GLU:HG3	1:B:240:ILE:CG2	2.47	0.45
1:A:368:LEU:O	1:A:372:VAL:HG13	2.17	0.44
1:B:24:GLU:OE2	1:B:27:LYS:HE3	2.17	0.44
1:B:385:GLU:HB2	1:B:388:MET:CE	2.46	0.44
1:B:13:SER:CB	1:B:115:ASP:OD2	2.65	0.44
1:A:362:CYS:SG	1:A:379:VAL:HG12	2.58	0.44
1:B:149:LEU:N	1:B:150:PRO:CD	2.82	0.43
1:B:378:ILE:HG13	1:B:423:LEU:HD22	1.99	0.43
1:A:81:HIS:CD2	1:B:306:HIS:HB3	2.54	0.43
1:B:196:LEU:HG	1:B:200:LYS:HE3	1.99	0.43
1:A:17:GLY:HA3	1:B:311:SER:HB2	2.01	0.42
1:B:268:PHE:CD1	1:B:349:VAL:HG11	2.54	0.42
1:A:179:ASP:OD1	1:A:387:ARG:HD2	2.18	0.42
1:B:152:LEU:HD12	1:B:152:LEU:HA	1.93	0.42
1:A:149:LEU:N	1:A:150:PRO:CD	2.82	0.42
1:B:362:CYS:SG	1:B:379:VAL:HG12	2.60	0.42
1:B:173:VAL:HG22	1:B:174:PRO:HD2	2.02	0.42
1:A:268:PHE:CD1	1:A:349:VAL:HG11	2.55	0.41
1:B:273:SER:CB	1:B:301:ARG:HH22	2.33	0.41
1:A:230:ASN:HB2	2:A:513:HOH:O	2.20	0.41
1:A:183:PRO:HB2	1:A:195:LEU:HD22	2.03	0.41
1:B:181:VAL:HG23	1:B:183:PRO:HD2	2.03	0.41
1:B:279:ASN:OD1	1:B:303:PRO:HG3	2.21	0.41
1:B:228:ASP:HA	1:B:229:PRO:HD2	1.98	0.41
1:A:318:GLN:HA	1:B:343:TRP:CD1	2.56	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	450/489 (92%)	443 (98%)	7 (2%)	0	100	100
1	B	445/489 (91%)	438 (98%)	7 (2%)	0	100	100
All	All	895/978 (92%)	881 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	393/425 (92%)	393 (100%)	0	100	100
1	B	389/425 (92%)	389 (100%)	0	100	100
All	All	782/850 (92%)	782 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	361	HIS
1	B	294	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 monosaccharides 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

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	454/489 (92%)	0.31	22 (4%) 30 37	27, 43, 76, 117	0
1	B	451/489 (92%)	0.40	32 (7%) 16 21	33, 52, 83, 112	0
All	All	905/978 (92%)	0.35	54 (5%) 21 28	27, 47, 82, 117	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	11.7
1	A	274	GLY	10.9
1	B	273	SER	4.5
1	A	273	SER	4.3
1	B	306	HIS	4.2
1	A	243	SER	4.1
1	B	76	PRO	4.1
1	B	106	GLN	3.7
1	A	407	GLN	3.4
1	A	304	ASN	3.1
1	B	312	PHE	3.1
1	A	22	LEU	3.0
1	A	115	ASP	3.0
1	B	407	GLN	3.0
1	A	306	HIS	3.0
1	A	466	GLN	2.8
1	B	427	ASP	2.8
1	A	312	PHE	2.7
1	B	21	PRO	2.7
1	A	34	HIS	2.6
1	B	304	ASN	2.6
1	B	259	ASP	2.6
1	B	115	ASP	2.6
1	B	226	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	365	ASN	2.5
1	B	263	SER	2.5
1	B	114	THR	2.5
1	A	108	GLN	2.5
1	A	303	PRO	2.5
1	A	136	PHE	2.4
1	B	75	LEU	2.4
1	A	408	ARG	2.4
1	A	114	THR	2.4
1	B	81	HIS	2.4
1	B	71	ASP	2.4
1	B	176	HIS	2.4
1	B	265	SER	2.3
1	B	262	PRO	2.3
1	A	210	VAL	2.3
1	B	156	VAL	2.3
1	A	463	LYS	2.3
1	B	20	ILE	2.2
1	B	165	GLU	2.2
1	B	73	ALA	2.2
1	A	307	SER	2.2
1	B	34	HIS	2.2
1	B	137	THR	2.1
1	A	19	LEU	2.1
1	B	255	LEU	2.1
1	B	434	TYR	2.1
1	A	11	VAL	2.0
1	A	137	THR	2.0
1	B	101	GLY	2.0
1	B	157	SER	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 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.