



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:39 PM BST

PDB ID : 6EJA
Title : Human Xylosyltransferase 1 in complex with peptide QEEEYSGGGQGG
Authors : Briggs, D.C.; Hohenester, E.
Deposited on : 2017-09-20
Resolution : 1.94 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

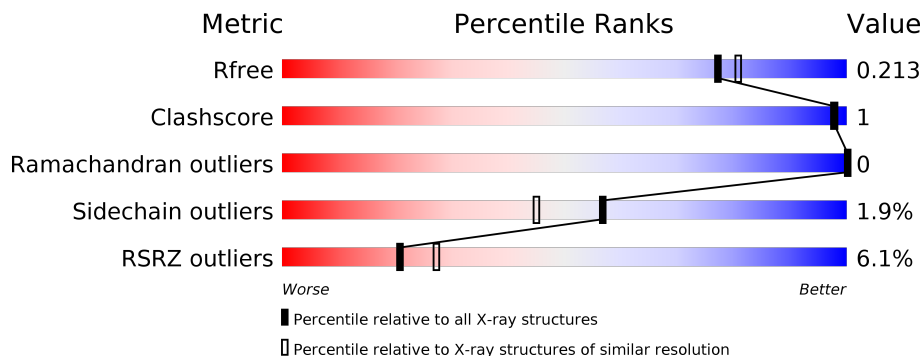
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 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	751	 6% 89% 7%
2	B	12	 8% 50% 8% 42%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11050 atoms, of which 5274 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 Xylosyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	696	10739	3524	5237	954	992	32	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ALA	-	expression tag	UNP Q86Y38
A	210	PRO	-	expression tag	UNP Q86Y38
A	211	LEU	-	expression tag	UNP Q86Y38
A	212	VAL	-	expression tag	UNP Q86Y38
A	213	HIS	-	expression tag	UNP Q86Y38
A	214	HIS	-	expression tag	UNP Q86Y38
A	215	HIS	-	expression tag	UNP Q86Y38
A	216	HIS	-	expression tag	UNP Q86Y38
A	217	HIS	-	expression tag	UNP Q86Y38
A	218	HIS	-	expression tag	UNP Q86Y38
A	219	ALA	-	expression tag	UNP Q86Y38
A	220	LEU	-	expression tag	UNP Q86Y38
A	221	ASP	-	expression tag	UNP Q86Y38
A	222	GLU	-	expression tag	UNP Q86Y38
A	223	ASN	-	expression tag	UNP Q86Y38
A	224	LEU	-	expression tag	UNP Q86Y38
A	225	TYR	-	expression tag	UNP Q86Y38
A	226	PHE	-	expression tag	UNP Q86Y38
A	227	GLN	-	expression tag	UNP Q86Y38
A	228	GLY	-	expression tag	UNP Q86Y38
A	229	ALA	-	expression tag	UNP Q86Y38
A	230	LEU	-	expression tag	UNP Q86Y38
A	231	ALA	-	expression tag	UNP Q86Y38

- Molecule 2 is a protein called Protein AMBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	7	85	28	37	8	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	214	TYR	GLY	engineered mutation	UNP P02760
B	220	GLY	LEU	engineered mutation	UNP P02760
B	221	GLY	VAL	engineered mutation	UNP P02760

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

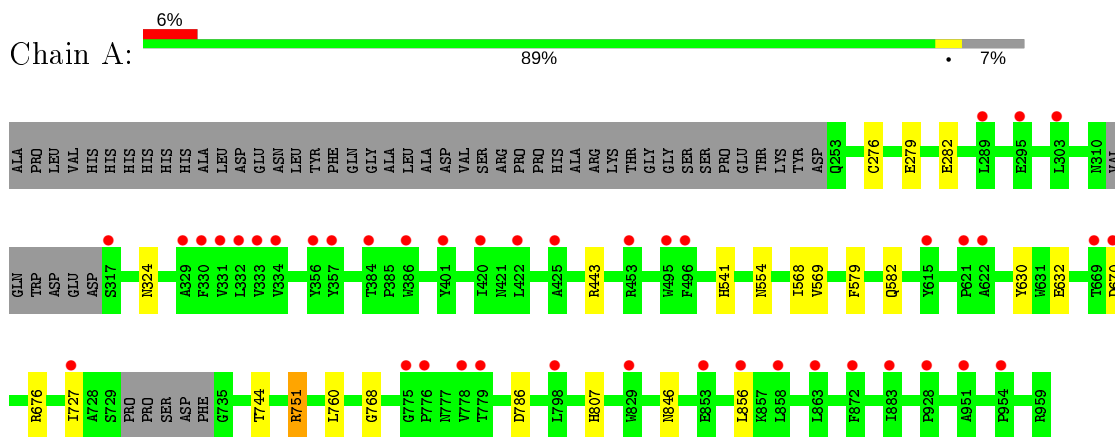
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		

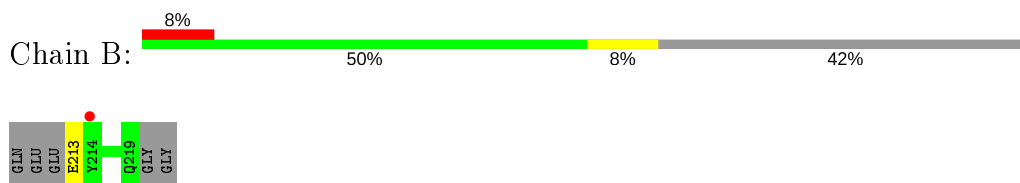
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Xylosyltransferase 1



- Molecule 2: Protein AMBP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.56Å 85.96Å 151.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.18 – 1.94 40.18 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.18-1.94) 98.8 (40.18-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.94Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.212 0.184 , 0.213	Depositor DCC
R_{free} test set	3183 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtrriage
Anisotropy	0.453	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11050	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.28	0/5663	0.48	0/7715
2	B	0.29	0/48	0.46	0/62
All	All	0.28	0/5711	0.48	0/7777

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

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	5502	5237	5233	7	1
2	B	48	37	36	0	0
3	A	1	0	0	0	0
4	A	225	0	0	1	0
All	All	5776	5274	5269	7	1

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 1.

All (7) 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:324:ASN:O	1:A:443:ARG:NH2	2.42	0.44
1:A:751:ARG:NE	4:A:1112:HOH:O	2.51	0.43
1:A:768:GLY:O	1:A:807:HIS:HA	2.18	0.43
1:A:568:ILE:HG22	1:A:569:VAL:HG13	2.02	0.41
1:A:630:TYR:CE2	1:A:632:GLU:HB2	2.56	0.40
1:A:554:ASN:HB2	1:A:579:PHE:CZ	2.56	0.40
1:A:744:THR:HG23	1:A:760:LEU:HD21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:HIS:HE2	1:A:670:ASP:OD1[1_545]	1.54	0.06

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	690/751 (92%)	675 (98%)	15 (2%)	0	100	100
2	B	5/12 (42%)	4 (80%)	1 (20%)	0	100	100
All	All	695/763 (91%)	679 (98%)	16 (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	577/656 (88%)	567 (98%)	10 (2%)	60	49
2	B	4/7 (57%)	3 (75%)	1 (25%)	0	0
All	All	581/663 (88%)	570 (98%)	11 (2%)	57	45

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	CYS
1	A	279	GLU
1	A	282	GLU
1	A	582	GLN
1	A	676	ARG
1	A	727	ILE
1	A	751	ARG
1	A	786	ASP
1	A	846	ASN
1	A	856	LEU
2	B	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 1 ligands modelled in this entry, 1 is 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

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	696/751 (92%)	0.54	42 (6%) 21 28	31, 49, 83, 112	0
2	B	7/12 (58%)	0.68	1 (14%) 2 3	52, 59, 78, 86	0
All	All	703/763 (92%)	0.54	43 (6%) 21 27	31, 49, 83, 112	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	863	LEU	5.3
1	A	829	TRP	4.8
1	A	289	LEU	4.0
1	A	856	LEU	3.8
1	A	858	LEU	3.7
1	A	401	TYR	3.6
1	A	420	ILE	3.2
1	A	954	PRO	3.2
1	A	669	THR	3.2
1	A	775	GLY	3.2
1	A	853	GLU	3.2
1	A	951	ALA	3.1
1	A	872	PHE	3.0
1	A	295	GLU	2.9
1	A	317	SER	2.9
1	A	357	TYR	2.8
1	A	622	ALA	2.8
1	A	883	ILE	2.8
1	A	670	ASP	2.7
2	B	214	TYR	2.6
1	A	303	LEU	2.6
1	A	495	TRP	2.6
1	A	776	PRO	2.6
1	A	333	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	330	PHE	2.5
1	A	332	LEU	2.5
1	A	928	PRO	2.5
1	A	779	THR	2.5
1	A	386	TRP	2.4
1	A	496	PHE	2.4
1	A	422	LEU	2.3
1	A	615	TYR	2.3
1	A	727	ILE	2.3
1	A	453	ARG	2.2
1	A	331	VAL	2.2
1	A	425	ALA	2.2
1	A	334	VAL	2.2
1	A	778	VAL	2.1
1	A	356	TYR	2.1
1	A	384	THR	2.1
1	A	329	ALA	2.1
1	A	621	PRO	2.0
1	A	798	LEU	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](#)

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, 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	B-factors(\AA^2)	Q<0.9
3	NA	A	1001	1/1	0.99	0.09	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.