



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2024 – 04:09 PM JST

PDB ID : 8XC8
Title : beta-1,4-galactosyltransferase
Authors : Luo, G.; Huang, Z.; Chen, J.; Hou, X.; Zhu, Y.; Ni, D.; Xu, W.; Zhang, W.;
Rao, Y.; Mu, W.
Deposited on : 2023-12-08
Resolution : 2.51 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

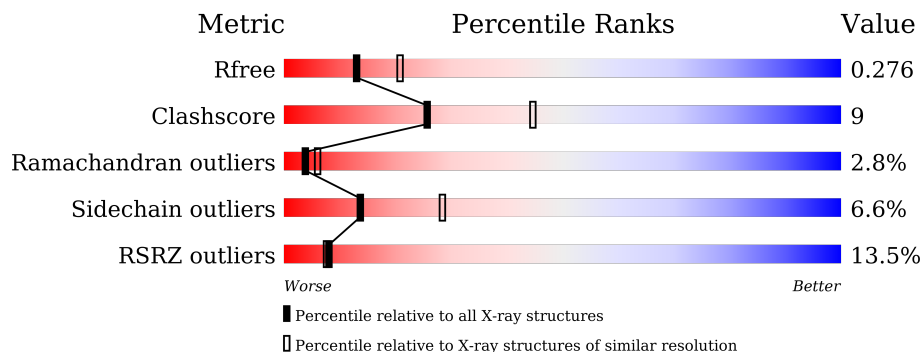
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	251	
1	B	251	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 3848 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 family 25 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	239	1967	1262	326	371	3	5	0	0	0
1	B	229	1875	1203	309	355	3	5	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	LYS	-	expression tag	UNP A0A5D0ENI3
A	234	ILE	-	expression tag	UNP A0A5D0ENI3
A	235	ASN	-	expression tag	UNP A0A5D0ENI3
A	236	LEU	-	expression tag	UNP A0A5D0ENI3
A	237	LYS	-	expression tag	UNP A0A5D0ENI3
A	238	TYR	-	expression tag	UNP A0A5D0ENI3
A	239	GLU	-	expression tag	UNP A0A5D0ENI3
A	240	LYS	-	expression tag	UNP A0A5D0ENI3
A	241	ARG	-	expression tag	UNP A0A5D0ENI3
A	242	LYS	-	expression tag	UNP A0A5D0ENI3
A	243	HIS	-	expression tag	UNP A0A5D0ENI3
A	244	LEU	-	expression tag	UNP A0A5D0ENI3
A	245	GLU	-	expression tag	UNP A0A5D0ENI3
A	246	HIS	-	expression tag	UNP A0A5D0ENI3
A	247	HIS	-	expression tag	UNP A0A5D0ENI3
A	248	HIS	-	expression tag	UNP A0A5D0ENI3
A	249	HIS	-	expression tag	UNP A0A5D0ENI3
A	250	HIS	-	expression tag	UNP A0A5D0ENI3
A	251	HIS	-	expression tag	UNP A0A5D0ENI3
B	233	LYS	-	expression tag	UNP A0A5D0ENI3
B	234	ILE	-	expression tag	UNP A0A5D0ENI3
B	235	ASN	-	expression tag	UNP A0A5D0ENI3
B	236	LEU	-	expression tag	UNP A0A5D0ENI3
B	237	LYS	-	expression tag	UNP A0A5D0ENI3
B	238	TYR	-	expression tag	UNP A0A5D0ENI3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	239	GLU	-	expression tag	UNP A0A5D0ENI3
B	240	LYS	-	expression tag	UNP A0A5D0ENI3
B	241	ARG	-	expression tag	UNP A0A5D0ENI3
B	242	LYS	-	expression tag	UNP A0A5D0ENI3
B	243	HIS	-	expression tag	UNP A0A5D0ENI3
B	244	LEU	-	expression tag	UNP A0A5D0ENI3
B	245	GLU	-	expression tag	UNP A0A5D0ENI3
B	246	HIS	-	expression tag	UNP A0A5D0ENI3
B	247	HIS	-	expression tag	UNP A0A5D0ENI3
B	248	HIS	-	expression tag	UNP A0A5D0ENI3
B	249	HIS	-	expression tag	UNP A0A5D0ENI3
B	250	HIS	-	expression tag	UNP A0A5D0ENI3
B	251	HIS	-	expression tag	UNP A0A5D0ENI3

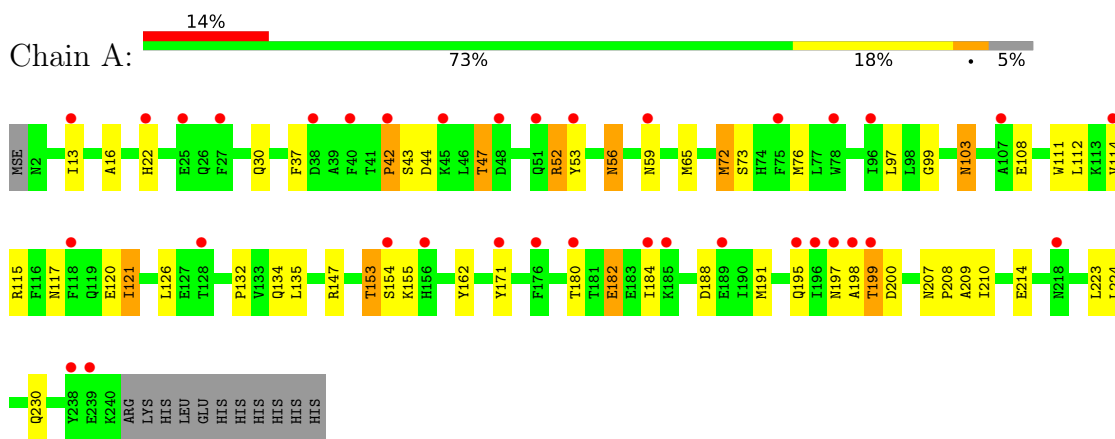
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	B	5	Total O 5 5	0	0

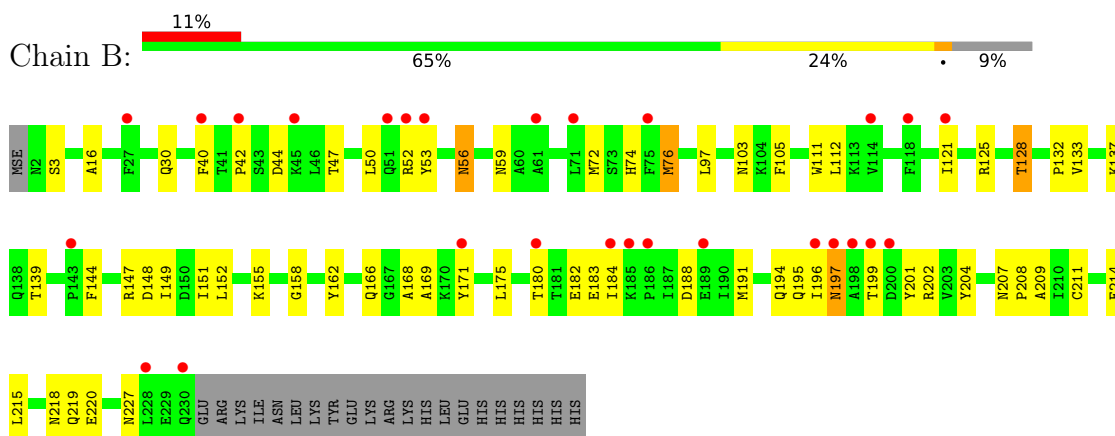
3 Residue-property plots [i](#)

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: Glycosyltransferase family 25 protein



- Molecule 1: Glycosyltransferase family 25 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.39Å 84.39Å 257.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.20 – 2.51 80.20 – 2.51	Depositor EDS
% Data completeness (in resolution range)	40.7 (80.20-2.51) 40.9 (80.20-2.51)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.236 , 0.279 0.250 , 0.276	Depositor DCC
R_{free} test set	1628 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3848	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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	0.62	0/2002	0.78	0/2699
1	B	0.63	0/1909	0.76	0/2577
All	All	0.63	0/3911	0.77	0/5276

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	1967	0	1945	40	0
1	B	1875	0	1844	40	0
2	A	1	0	0	0	0
2	B	5	0	0	0	0
All	All	3848	0	3789	72	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 9.

The worst 5 of 72 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:B:72:MSE:SE	1:B:76:MSE:HE3	1.76	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:MSE:SE	1:B:76:MSE:CE	2.67	0.93
1:B:139:THR:HG21	1:B:149:ILE:O	1.75	0.86
1:B:132:PRO:HD3	1:B:219:GLN:HE22	1.60	0.66
1:B:182:GLU:HG3	1:B:183:GLU:OE1	1.94	0.65

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	237/251 (94%)	194 (82%)	37 (16%)	6 (2%)	4	7
1	B	227/251 (90%)	192 (85%)	28 (12%)	7 (3%)	3	5
All	All	464/502 (92%)	386 (83%)	65 (14%)	13 (3%)	4	6

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	B	56	ASN
1	A	199	THR
1	A	16	ALA
1	B	16	ALA

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	218/224 (97%)	203 (93%)	15 (7%)	13	26
1	B	208/224 (93%)	195 (94%)	13 (6%)	15	30
All	All	426/448 (95%)	398 (93%)	28 (7%)	14	28

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

Mol	Chain	Res	Type
1	A	197	ASN
1	B	227	ASN
1	B	47	THR
1	B	215	LEU
1	B	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	B	219	GLN
1	A	216	GLN
1	A	219	GLN
1	B	21	ASN

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	234/251 (93%)	1.03	35 (14%) 6 6	41, 76, 121, 184	0
1	B	224/251 (89%)	0.92	27 (12%) 10 9	39, 73, 117, 136	0
All	All	458/502 (91%)	0.98	62 (13%) 8 7	39, 75, 121, 184	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	7.7
1	A	180	THR	5.7
1	A	198	ALA	4.8
1	A	154	SER	4.3
1	B	185	LYS	4.3

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.