



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 6EOU / pdb_00006eou
Title : O-GlcNAc transferase TPR domain with the intellectual disability associated mutation L254F
Authors : Gundogdu, M.; van Aalten, D.M.F.
Deposited on : 2017-10-10
Resolution : 1.75 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

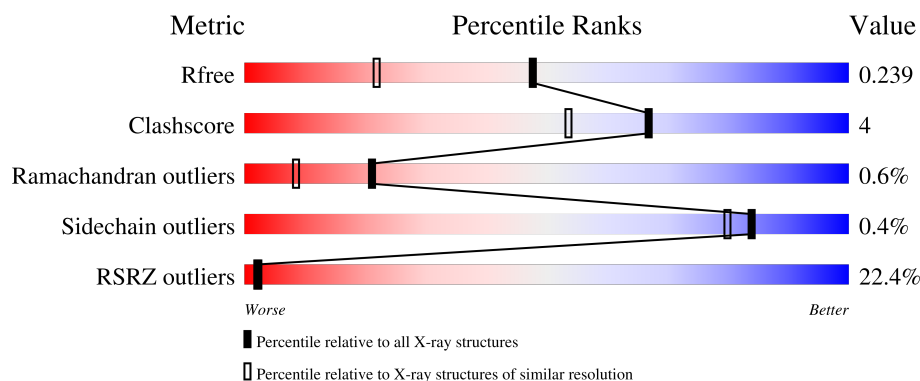
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	388	20% 73% 15% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2988 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 UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	3	0
			2708	1722	475	501	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP O15294
A	24	PRO	-	expression tag	UNP O15294
A	25	MET	-	expression tag	UNP O15294
A	254	PHE	LEU	engineered mutation	UNP O15294

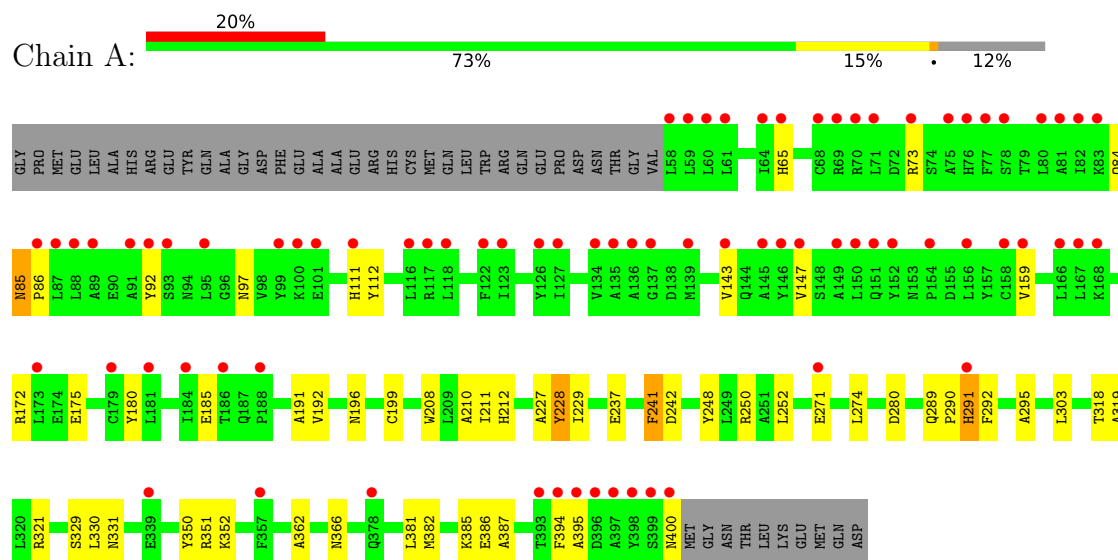
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	280	Total	O	0	0
			280	280		

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: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	45.00Å 203.16Å 116.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.58 – 1.75 101.58 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (101.58-1.75) 99.5 (101.58-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.191 , 0.227 0.203 , 0.239	Depositor DCC
R_{free} test set	2582 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2988	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	1.61	31/2780 (1.1%)	1.28	6/3776 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	ASN	CG-OD1	-8.31	1.07	1.23
1	A	228	TYR	N-CA	8.10	1.56	1.46
1	A	237	GLU	N-CA	7.63	1.55	1.46
1	A	211	ILE	CA-CB	7.63	1.63	1.54
1	A	210	ALA	N-CA	7.39	1.55	1.46
1	A	321	ARG	N-CA	7.32	1.55	1.46
1	A	229	ILE	N-CA	-7.20	1.38	1.46
1	A	248	TYR	CA-CB	-7.08	1.42	1.53
1	A	212	HIS	CA-C	6.83	1.61	1.52
1	A	381	LEU	N-CA	-6.71	1.38	1.46
1	A	303	LEU	C-O	6.63	1.31	1.24
1	A	227	ALA	CA-CB	-6.42	1.43	1.53
1	A	362	ALA	CA-C	-6.36	1.44	1.52
1	A	242	ASP	CG-OD1	6.31	1.37	1.25
1	A	208	TRP	N-CA	-6.25	1.38	1.46
1	A	319	ALA	CA-C	6.24	1.60	1.52
1	A	210	ALA	CA-C	-6.15	1.45	1.52
1	A	199	CYS	N-CA	-6.12	1.38	1.46
1	A	252	LEU	CA-CB	-5.97	1.43	1.53
1	A	387	ALA	N-CA	5.87	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	LYS	C-O	-5.73	1.17	1.24
1	A	241	PHE	CA-CB	-5.51	1.44	1.53
1	A	386	GLU	CA-C	5.51	1.60	1.52
1	A	329	SER	N-CA	-5.48	1.39	1.46
1	A	351	ARG	N-CA	-5.45	1.39	1.46
1	A	192	VAL	CA-C	-5.41	1.45	1.52
1	A	295	ALA	N-CA	5.33	1.53	1.46
1	A	395	ALA	N-CA	5.32	1.52	1.46
1	A	274	LEU	N-CA	-5.18	1.40	1.46
1	A	191	ALA	N-CA	5.04	1.52	1.46
1	A	159	VAL	CA-C	-5.02	1.46	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASN	N-CA-C	6.06	117.89	111.28
1	A	212	HIS	O-C-N	5.51	127.82	122.09
1	A	318	THR	N-CA-C	5.43	117.20	111.28
1	A	330	LEU	N-CA-C	5.33	116.78	111.07
1	A	385	LYS	N-CA-C	5.25	117.74	111.71
1	A	290	PRO	CB-CA-C	-5.07	103.73	110.27

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291[B]	HIS	Peptide

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	2708	0	2649	20	0
2	A	280	0	0	7	1
All	All	2988	0	2649	20	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 4.

All (20) 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:289:GLN:HG2	2:A:736:HOH:O	1.60	1.01
1:A:382:MET:HB3	2:A:726:HOH:O	1.62	0.98
1:A:394:PHE:HA	2:A:663:HOH:O	1.71	0.91
1:A:241:PHE:CZ	1:A:271:GLU:HG2	2.07	0.88
1:A:280[A]:ASP:OD1	2:A:501:HOH:O	2.11	0.69
1:A:280[B]:ASP:OD1	2:A:502:HOH:O	2.16	0.59
1:A:241:PHE:CZ	1:A:271:GLU:CG	2.89	0.53
1:A:228:TYR:CE1	1:A:250:ARG:HG2	2.47	0.49
1:A:84:GLN:O	1:A:85:ASN:HB2	2.12	0.49
1:A:228:TYR:CZ	1:A:250:ARG:HG2	2.47	0.49
1:A:143:VAL:O	1:A:147:VAL:HG23	2.13	0.48
1:A:350:TYR:CZ	1:A:366:ASN:HB3	2.48	0.48
1:A:292:PHE:HA	2:A:541:HOH:O	2.14	0.47
1:A:180:TYR:CZ	1:A:196:ASN:HB3	2.49	0.47
1:A:65:HIS:CD2	1:A:73:ARG:HB3	2.53	0.44
1:A:289:GLN:OE1	1:A:291[B]:HIS:ND1	2.49	0.44
1:A:352:LYS:NZ	2:A:516:HOH:O	2.51	0.43
1:A:97:ASN:ND2	1:A:112:TYR:OH	2.46	0.42
1:A:92:TYR:O	1:A:111:HIS:HB3	2.20	0.42
1:A:172:ARG:NH1	1:A:175:GLU:OE1	2.53	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)
2:A:665:HOH:O	2:A:726:HOH:O[1_455]	2.13	0.07

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	344/388 (89%)	338 (98%)	4 (1%)	2 (1%)	21 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	86	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	278/314 (88%)	277 (100%)	1 (0%)	84 80

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	97	ASN
1	A	128	ASN
1	A	202	ASN
1	A	223	ASN
1	A	272	GLN
1	A	374	GLN

5.3.3 RNA ⓘ

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 ⓘ

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	343/388 (88%)	1.04	77 (22%) 2 2	12, 35, 73, 93	2 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	LEU	6.2
1	A	59	LEU	4.7
1	A	88	LEU	4.7
1	A	397	ALA	4.7
1	A	58	LEU	4.5
1	A	77	PHE	4.4
1	A	73	ARG	4.2
1	A	80	LEU	4.1
1	A	394	PHE	4.0
1	A	61	LEU	4.0
1	A	291[A]	HIS	4.0
1	A	395	ALA	4.0
1	A	87	LEU	3.9
1	A	118	LEU	3.8
1	A	81	ALA	3.8
1	A	136	ALA	3.7
1	A	93	SER	3.5
1	A	83	LYS	3.3
1	A	123	ILE	3.2
1	A	139	MET	3.2
1	A	82	ILE	3.1
1	A	71	LEU	3.1
1	A	398	TYR	3.0
1	A	95	LEU	3.0
1	A	134	VAL	3.0
1	A	89	ALA	3.0
1	A	116	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	396	ASP	2.9
1	A	76	HIS	2.9
1	A	64	ILE	2.9
1	A	147	VAL	2.8
1	A	100	LYS	2.8
1	A	156	LEU	2.8
1	A	173	LEU	2.8
1	A	78	SER	2.8
1	A	68	CYS	2.8
1	A	393	THR	2.8
1	A	137	GLY	2.8
1	A	152	TYR	2.7
1	A	186	THR	2.7
1	A	181	LEU	2.6
1	A	143	VAL	2.6
1	A	145	ALA	2.6
1	A	150	LEU	2.5
1	A	126	TYR	2.5
1	A	154	PRO	2.5
1	A	151	GLN	2.5
1	A	122	PHE	2.5
1	A	86	PRO	2.5
1	A	99	TYR	2.5
1	A	69	ARG	2.5
1	A	167	LEU	2.4
1	A	127	ILE	2.4
1	A	378	GLN	2.4
1	A	271	GLU	2.4
1	A	75	ALA	2.4
1	A	65	HIS	2.4
1	A	166	LEU	2.4
1	A	101	GLU	2.4
1	A	339	GLU	2.4
1	A	399	SER	2.3
1	A	188	PRO	2.3
1	A	158	CYS	2.3
1	A	357[A]	PHE	2.3
1	A	92	TYR	2.3
1	A	179	CYS	2.3
1	A	168	LYS	2.2
1	A	159	VAL	2.2
1	A	135	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	91	ALA	2.1
1	A	184	ILE	2.1
1	A	149	ALA	2.1
1	A	400	ASN	2.1
1	A	117	ARG	2.0
1	A	70	ARG	2.0
1	A	146	TYR	2.0
1	A	111	HIS	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.