



wwPDB X-ray Structure Validation Summary Report i

Nov 26, 2014 – 10:52 PM EST

PDB ID : 3WZT
Title : Crystal structure of Trx3 domain of UGGT (detergent-unbound form)
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Deposited on : 2014-10-03
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

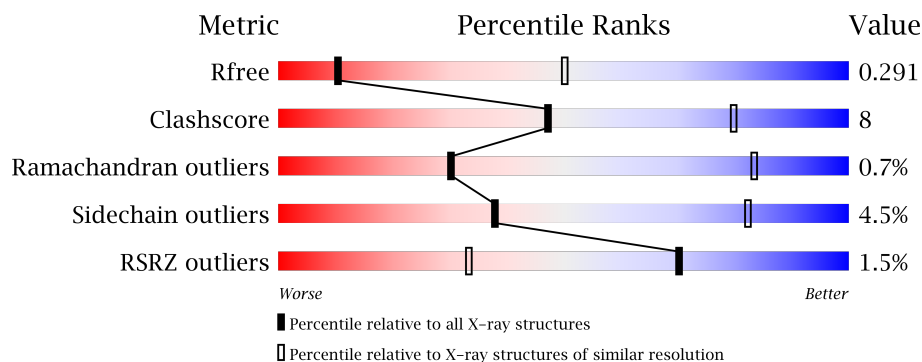
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24195
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24195

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	163	
1	B	163	
1	C	163	
1	D	163	
1	E	163	
1	F	163	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6452 atoms, of which 0 are hydrogen and 0 are deuterium.

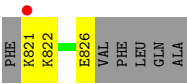
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UDP-glucose-glycoproteinglucosyltransferase-likeprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	Se	0	0	0
			1239	783	208	246	2			
1	B	156	Total	C	N	O	Se	0	0	0
			1246	788	209	247	2			
1	C	142	Total	C	N	O	Se	0	0	0
			1127	715	189	221	2			
1	D	154	Total	C	N	O	Se	0	0	0
			1231	779	206	244	2			
1	E	94	Total	C	N	O	Se	0	0	0
			738	469	122	145	2			
1	F	111	Total	C	N	O	Se	0	0	0
			871	552	150	168	1			

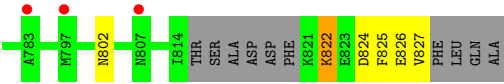
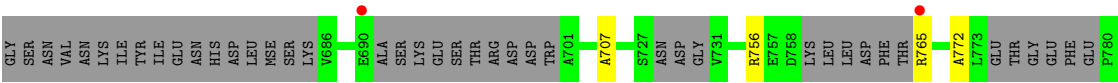
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	669	GLY	-	EXPRESSION TAG	UNP G0SB58
A	670	SER	-	EXPRESSION TAG	UNP G0SB58
B	669	GLY	-	EXPRESSION TAG	UNP G0SB58
B	670	SER	-	EXPRESSION TAG	UNP G0SB58
C	669	GLY	-	EXPRESSION TAG	UNP G0SB58
C	670	SER	-	EXPRESSION TAG	UNP G0SB58
D	669	GLY	-	EXPRESSION TAG	UNP G0SB58
D	670	SER	-	EXPRESSION TAG	UNP G0SB58
E	669	GLY	-	EXPRESSION TAG	UNP G0SB58
E	670	SER	-	EXPRESSION TAG	UNP G0SB58
F	669	GLY	-	EXPRESSION TAG	UNP G0SB58
F	670	SER	-	EXPRESSION TAG	UNP G0SB58



● Molecule 1: UDP-glucose-glycoproteinglucosyltransferase-likeprotein

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	196.40Å 196.40Å 196.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 19.84 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.40) 100.0 (19.84-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.39 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.235 , 0.292 0.235 , 0.291	Depositor DCC
R_{free} test set	865 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.5	EDS
Estimated twinning fraction	0.022 for -l,-k,-h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17343 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6452	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.54	0/1257	0.69	2/1695 (0.1%)
1	B	0.55	0/1264	0.69	1/1705 (0.1%)
1	C	0.53	0/1143	0.74	4/1541 (0.3%)
1	D	0.53	0/1249	0.67	0/1684
1	E	0.54	0/742	0.69	0/993
1	F	0.43	0/878	0.63	0/1179
All	All	0.53	0/6533	0.69	7/8797 (0.1%)

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
1	E	0	6
All	All	0	7

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	797	MSE	CA-CB-CG	8.07	127.01	113.30
1	A	765	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	C	803	PHE	CB-CA-C	-5.77	98.85	110.40
1	A	765	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	803	PHE	CB-CG-CD1	5.17	124.42	120.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	673	ASN	Peptide
1	E	705	VAL	Peptide
1	E	733	LEU	Peptide
1	E	782	VAL	Peptide
1	E	783	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1239	0	1216	12	0
1	B	1246	0	1225	16	0
1	C	1127	0	1107	25	0
1	D	1231	0	1210	42	0
1	E	738	0	731	33	0
1	F	871	0	877	4	0
All	All	6452	0	6366	102	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 102 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:782:VAL:CG2	1:D:812:GLY:HA2	1.80	1.10
1:B:782:VAL:HG21	1:D:812:GLY:HA2	1.33	1.09
1:D:700:TRP:HH2	1:E:783:ALA:H	1.11	0.96
1:D:700:TRP:HH2	1:E:783:ALA:N	1.62	0.96
1:B:782:VAL:CG2	1:D:812:GLY:CA	2.56	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	151/163 (93%)	142 (94%)	9 (6%)	0	100	100
1	B	152/163 (93%)	146 (96%)	6 (4%)	0	100	100
1	C	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
1	D	150/163 (92%)	143 (95%)	7 (5%)	0	100	100
1	E	80/163 (49%)	66 (82%)	9 (11%)	5 (6%)	2	27
1	F	99/163 (61%)	96 (97%)	3 (3%)	0	100	100
All	All	768/978 (78%)	722 (94%)	41 (5%)	5 (1%)	30	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	708	ASP
1	E	807	ASN
1	E	789	ALA
1	E	748	VAL
1	E	687	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	137/140 (98%)	131 (96%)	6 (4%)	39	83
1	B	138/140 (99%)	133 (96%)	5 (4%)	47	86
1	C	124/140 (89%)	117 (94%)	7 (6%)	30	75
1	D	136/140 (97%)	130 (96%)	6 (4%)	39	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	83/140 (59%)	78 (94%)	5 (6%)	27	73
1	F	96/140 (69%)	93 (97%)	3 (3%)	52	90
All	All	714/840 (85%)	682 (96%)	32 (4%)	38	82

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	774	GLU
1	C	826	GLU
1	F	765	ARG
1	C	822	LYS
1	D	681	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	728	ASN
1	D	680	HIS
1	D	728	ASN
1	E	796	ASN
1	E	807	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	155/163 (95%)	-0.09	1 (0%) 86 55	50, 73, 115, 176	0
1	B	156/163 (95%)	-0.12	1 (0%) 86 55	52, 75, 112, 167	0
1	C	142/163 (87%)	-0.04	0 100 100	59, 87, 123, 155	0
1	D	154/163 (94%)	0.02	2 (1%) 74 37	55, 89, 146, 179	0
1	E	94/163 (57%)	0.44	3 (3%) 45 18	99, 132, 171, 190	0
1	F	111/163 (68%)	0.63	5 (4%) 32 12	100, 139, 165, 189	0
All	All	812/978 (83%)	0.09	12 (1%) 70 33	50, 91, 155, 190	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	690	GLU	4.5
1	D	693	LYS	3.7
1	E	821	LYS	2.9
1	B	696	THR	2.7
1	E	720	TYR	2.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.