



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:55 AM GMT

PDB ID : 4BCE
Title : crystal structure of Ttb-gly N282T mutant
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Deposited on : 2012-10-02
Resolution : 2.00 Å(reported)

This is a full wwPDB validation 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>

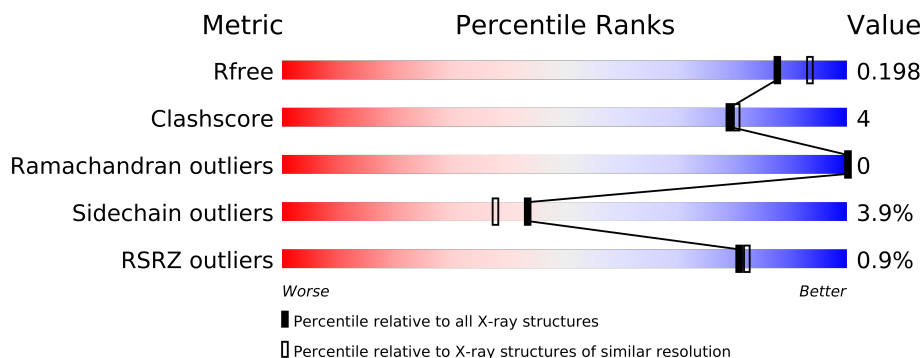
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	437	
1	B	437	
1	C	437	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10817 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 BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	3	0
			3430	2209	617	599	5			
1	B	425	Total	C	N	O	S	0	1	0
			3427	2207	615	600	5			
1	C	424	Total	C	N	O	S	0	2	0
			3417	2202	610	600	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	HIS	-	EXPRESSION TAG	UNP Q53W75
A	433	HIS	-	EXPRESSION TAG	UNP Q53W75
A	434	HIS	-	EXPRESSION TAG	UNP Q53W75
A	435	HIS	-	EXPRESSION TAG	UNP Q53W75
A	436	HIS	-	EXPRESSION TAG	UNP Q53W75
A	437	HIS	-	EXPRESSION TAG	UNP Q53W75
A	282	THR	ASN	ENGINEERED MUTATION	UNP Q53W75
A	320	HIS	TYR	ENGINEERED MUTATION	UNP Q53W75
B	432	HIS	-	EXPRESSION TAG	UNP Q53W75
B	433	HIS	-	EXPRESSION TAG	UNP Q53W75
B	434	HIS	-	EXPRESSION TAG	UNP Q53W75
B	435	HIS	-	EXPRESSION TAG	UNP Q53W75
B	436	HIS	-	EXPRESSION TAG	UNP Q53W75
B	437	HIS	-	EXPRESSION TAG	UNP Q53W75
B	282	THR	ASN	ENGINEERED MUTATION	UNP Q53W75
B	320	HIS	TYR	ENGINEERED MUTATION	UNP Q53W75
C	432	HIS	-	EXPRESSION TAG	UNP Q53W75
C	433	HIS	-	EXPRESSION TAG	UNP Q53W75
C	434	HIS	-	EXPRESSION TAG	UNP Q53W75
C	435	HIS	-	EXPRESSION TAG	UNP Q53W75
C	436	HIS	-	EXPRESSION TAG	UNP Q53W75
C	437	HIS	-	EXPRESSION TAG	UNP Q53W75
C	282	THR	ASN	ENGINEERED MUTATION	UNP Q53W75

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Chain	Residue	Modelled	Actual	Comment	Reference
C	320	HIS	TYR	ENGINEERED MUTATION	UNP Q53W75

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	223	Total 224	O 224	0	1
2	B	187	Total 187	O 187	0	0
2	C	132	Total 132	O 132	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.17Å 77.67Å 122.02Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	39.97 – 2.00 39.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.97-2.00) 99.3 (39.97-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.190 0.174 , 0.198	Depositor DCC
R_{free} test set	4438 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 29.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 88517 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10817	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	1.34	18/3542 (0.5%)	1.11	10/4831 (0.2%)
1	B	1.33	11/3539 (0.3%)	1.08	11/4828 (0.2%)
1	C	1.22	10/3529 (0.3%)	0.98	9/4815 (0.2%)
All	All	1.30	39/10610 (0.4%)	1.06	30/14474 (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	B	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	GLU	CG-CD	11.73	1.69	1.51
1	A	424	GLU	CD-OE1	10.09	1.36	1.25
1	C	204	GLU	CG-CD	9.38	1.66	1.51
1	C	204	GLU	CD-OE1	9.32	1.35	1.25
1	B	424	GLU	CD-OE1	9.23	1.35	1.25
1	A	204	GLU	CD-OE1	8.63	1.35	1.25
1	B	424	GLU	CG-CD	8.53	1.64	1.51
1	C	424	GLU	CG-CD	8.29	1.64	1.51
1	A	204	GLU	CG-CD	8.28	1.64	1.51
1	B	204	GLU	CD-OE1	7.80	1.34	1.25
1	A	294	GLY	N-CA	7.34	1.57	1.46
1	A	270	GLU	CG-CD	6.99	1.62	1.51
1	A	204	GLU	CB-CG	6.93	1.65	1.52
1	B	204	GLU	CG-CD	6.91	1.62	1.51
1	C	204	GLU	CB-CG	6.79	1.65	1.52
1	B	392	GLU	CG-CD	6.65	1.61	1.51
1	C	136	GLU	CG-CD	6.59	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	GLU	CG-CD	6.37	1.61	1.51
1	A	338	GLU	CD-OE1	6.16	1.32	1.25
1	A	226	GLU	CG-CD	6.07	1.61	1.51
1	B	204	GLU	CB-CG	5.81	1.63	1.52
1	A	74	TYR	CE1-CZ	-5.72	1.31	1.38
1	B	136	GLU	CD-OE1	5.68	1.31	1.25
1	B	329	GLU	CB-CG	-5.68	1.41	1.52
1	A	328	ARG	CG-CD	5.64	1.66	1.51
1	A	204	GLU	CD-OE2	5.61	1.31	1.25
1	C	237	TYR	CE1-CZ	5.57	1.45	1.38
1	B	71	VAL	CB-CG1	-5.53	1.41	1.52
1	A	300	TYR	CG-CD2	5.42	1.46	1.39
1	B	120	TRP	CD2-CE2	5.37	1.47	1.41
1	C	204	GLU	CD-OE2	5.31	1.31	1.25
1	C	424	GLU	CD-OE1	5.27	1.31	1.25
1	C	125	ALA	CA-CB	5.26	1.63	1.52
1	A	213	ARG	CG-CD	-5.23	1.38	1.51
1	A	329	GLU	CG-CD	5.17	1.59	1.51
1	A	328	ARG	CZ-NH2	5.17	1.39	1.33
1	A	338	GLU	CG-CD	5.16	1.59	1.51
1	C	33	TRP	CE3-CZ3	5.04	1.47	1.38
1	B	166	TRP	CE3-CZ3	5.02	1.47	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH2	-13.23	113.69	120.30
1	A	293	THR	C-N-CA	-10.81	99.60	122.30
1	B	75	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	A	373	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	C	207	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	425	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	C	28	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	B	72	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	C	28	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	96	LEU	CB-CG-CD1	6.44	121.94	111.00
1	B	213	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	C	133	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	373	ARG	CG-CD-NE	-6.15	98.88	111.80
1	B	154	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	135	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	154	ASP	CB-CG-OD1	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	399	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	82	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	328	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	96	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	C	88	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	121	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	373	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	378	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	240	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	57	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	424	GLU	CG-CD-OE1	5.16	128.62	118.30
1	B	417	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	293	THR	O-C-N	-5.09	114.54	123.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	ASN	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	3430	0	0	14	0
1	B	3427	0	0	8	0
1	C	3417	0	0	14	0
2	A	224	0	0	3	0
2	B	187	0	0	4	0
2	C	132	0	0	5	0
All	All	10817	0	0	36	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 4.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:129:ARG:NH1	2:C:2059:HOH:O	1.74	1.18
1:B:129:ARG:NH1	1:B:136:GLU:OE1	2.05	0.90
1:C:101[B]:ARG:CG	1:C:101[B]:ARG:NH1	2.42	0.79
1:C:425:ARG:NH1	2:C:2116:HOH:O	2.17	0.78
1:A:266:SER:O	1:A:267[B]:ARG:CB	2.27	0.78
1:B:392:GLU:OE1	2:B:2185:HOH:O	2.06	0.73
1:C:101[B]:ARG:CZ	2:C:2051:HOH:O	2.37	0.73
1:A:282:THR:OG1	2:A:2104:HOH:O	2.11	0.68
1:B:282:THR:OG1	2:B:2088:HOH:O	2.13	0.67
1:A:423:ARG:CG	1:A:423:ARG:NH1	2.59	0.65
1:A:224:TYR:OH	1:A:321:HIS:CD2	2.52	0.61
1:A:392:GLU:OE1	2:A:2221:HOH:O	2.16	0.61
1:A:59:TYR:OH	1:A:101[A]:ARG:NE	2.36	0.59
1:A:59:TYR:OH	1:A:101[B]:ARG:NE	2.36	0.59
1:C:348:THR:N	1:C:350:GLU:OE2	2.42	0.53
1:C:308:THR:O	1:C:311:GLY:N	2.42	0.51
1:B:55:HIS:CD2	1:B:62:ASP:OD2	2.65	0.49
1:A:424:GLU:OE2	1:A:428:ARG:NH2	2.45	0.49
1:B:7:LYS:O	2:B:2003:HOH:O	2.20	0.49
1:C:257:ARG:CD	2:C:2096:HOH:O	2.60	0.49
1:A:59:TYR:OH	1:A:101[A]:ARG:CD	2.61	0.48
1:A:59:TYR:OH	1:A:101[B]:ARG:CD	2.61	0.48
1:C:127:GLU:OE2	1:C:133:ARG:NH1	2.47	0.48
1:A:58:ARG:NH1	2:A:2048:HOH:O	2.47	0.47
1:C:55:HIS:CD2	1:C:62:ASP:OD2	2.68	0.47
1:B:345:ASP:OD2	1:B:416:LYS:NZ	2.49	0.46
1:C:101[B]:ARG:NH2	2:C:2051:HOH:O	2.49	0.43
1:C:130:GLY:O	1:C:131:GLY:C	2.56	0.43
1:C:80:TRP:N	1:C:81:PRO:CD	2.82	0.42
1:B:194:HIS:CE1	2:B:2076:HOH:O	2.72	0.42
1:C:290:ALA:O	1:C:299:ARG:N	2.53	0.42
1:C:267:ARG:NH1	1:C:270:GLU:OE1	2.54	0.41
1:B:80:TRP:N	1:B:81:PRO:CD	2.83	0.41
1:A:266:SER:O	1:A:267[A]:ARG:CB	2.67	0.40
1:A:100:ASP:OD1	1:A:155:ARG:NH2	2.54	0.40
1:A:72:ARG:NH2	1:A:110:GLY:O	2.55	0.40

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	425/437 (97%)	414 (97%)	11 (3%)	0	100	100
1	B	425/437 (97%)	410 (96%)	15 (4%)	0	100	100
1	C	424/437 (97%)	407 (96%)	17 (4%)	0	100	100
All	All	1274/1311 (97%)	1231 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	336/345 (97%)	322 (96%)	14 (4%)	40	34
1	B	336/345 (97%)	325 (97%)	11 (3%)	50	46
1	C	335/345 (97%)	320 (96%)	15 (4%)	38	31
All	All	1007/1035 (97%)	967 (96%)	40 (4%)	43	36

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	51	PRO
1	A	61	GLU
1	A	82	ARG
1	A	84	LEU
1	A	96	LEU
1	A	257[A]	ARG
1	A	257[B]	ARG

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Mol	Chain	Res	Type
1	A	298	VAL
1	A	328	ARG
1	A	346	LEU
1	A	423	ARG
1	A	424	GLU
1	A	425	ARG
1	B	7	LYS
1	B	61	GLU
1	B	100	ASP
1	B	105	ARG
1	B	107	LEU
1	B	257	ARG
1	B	266	SER
1	B	346	LEU
1	B	420	LEU
1	B	424	GLU
1	B	425	ARG
1	C	6	GLU
1	C	44	ARG
1	C	51	PRO
1	C	61	GLU
1	C	72	ARG
1	C	82	ARG
1	C	128	GLU
1	C	133	ARG
1	C	226	GLU
1	C	229	GLU
1	C	266	SER
1	C	267	ARG
1	C	304	GLU
1	C	325	ARG
1	C	425	ARG

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

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	424/437 (97%)	-0.55	1 (0%) 93 94	14, 27, 46, 67	0
1	B	425/437 (97%)	-0.49	6 (1%) 72 72	14, 29, 51, 72	0
1	C	424/437 (97%)	-0.06	5 (1%) 75 76	23, 38, 67, 84	0
All	All	1273/1311 (97%)	-0.37	12 (0%) 81 82	14, 31, 58, 84	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	ARG	3.3
1	C	226	GLU	2.9
1	A	304	GLU	2.8
1	B	293	THR	2.8
1	B	90	ARG	2.7
1	C	304	GLU	2.3
1	C	228	PRO	2.3
1	B	299	ARG	2.2
1	B	6	GLU	2.1
1	B	261	PRO	2.1
1	C	257	ARG	2.1
1	B	257	ARG	2.0

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.