



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:28 PM EDT

PDB ID : 8DFX / pdb_00008dfx
Title : Crystal structure of Human BTN2A1-BTN3A1 Ectodomain Complex
Authors : Fulford, T.S.; Soliman, C.; Castle, R.G.; Rigau, M.; Ruan, Z.; Dolezal, O.; Seneviratna, R.; Brown, H.G.; Hanssen, E.; Hammet, A.; Li, S.; Redmond, S.J.; Chung, A.; Gorman, M.A.; Parker, M.W.; Patel, O.; Peat, T.S.; Newman, J.; Behren, A.; Gherardin, N.A.; Godfrey, D.I.; Uldrich, A.P.
Deposited on : 2022-06-22
Resolution : 5.55 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 : **FAILED**
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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 5.55 Å.

There are no overall percentile quality scores available for this entry.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3305 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1695	1069	297	318	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	expression tag	UNP Q7KYR7
A	-1	THR	-	expression tag	UNP Q7KYR7
A	0	GLY	-	expression tag	UNP Q7KYR7
A	218	HIS	-	expression tag	UNP Q7KYR7
A	219	HIS	-	expression tag	UNP Q7KYR7
A	220	HIS	-	expression tag	UNP Q7KYR7
A	221	HIS	-	expression tag	UNP Q7KYR7
A	222	HIS	-	expression tag	UNP Q7KYR7
A	223	HIS	-	expression tag	UNP Q7KYR7

- Molecule 2 is a protein called Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1582	1000	269	305	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLU	-	expression tag	UNP O00481
B	-1	THR	-	expression tag	UNP O00481
B	0	GLY	-	expression tag	UNP O00481
B	218	SER	-	expression tag	UNP O00481
B	219	GLY	-	expression tag	UNP O00481
B	220	GLY	-	expression tag	UNP O00481
B	221	LEU	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	THR	-	expression tag	UNP O00481
B	223	PRO	-	expression tag	UNP O00481
B	224	ARG	-	expression tag	UNP O00481
B	225	GLY	-	expression tag	UNP O00481
B	226	VAL	-	expression tag	UNP O00481
B	227	ARG	-	expression tag	UNP O00481
B	228	LEU	-	expression tag	UNP O00481
B	229	GLY	-	expression tag	UNP O00481
B	230	GLY	-	expression tag	UNP O00481
B	231	LEU	-	expression tag	UNP O00481
B	232	GLU	-	expression tag	UNP O00481
B	233	ILE	-	expression tag	UNP O00481
B	234	ARG	-	expression tag	UNP O00481
B	235	ALA	-	expression tag	UNP O00481
B	236	ALA	-	expression tag	UNP O00481
B	237	PHE	-	expression tag	UNP O00481
B	238	LEU	-	expression tag	UNP O00481
B	239	ARG	-	expression tag	UNP O00481
B	240	ARG	-	expression tag	UNP O00481
B	241	ARG	-	expression tag	UNP O00481
B	242	ASN	-	expression tag	UNP O00481
B	243	THR	-	expression tag	UNP O00481
B	244	ALA	-	expression tag	UNP O00481
B	245	LEU	-	expression tag	UNP O00481
B	246	ARG	-	expression tag	UNP O00481
B	247	THR	-	expression tag	UNP O00481
B	248	ARG	-	expression tag	UNP O00481
B	249	VAL	-	expression tag	UNP O00481
B	250	ALA	-	expression tag	UNP O00481
B	251	GLU	-	expression tag	UNP O00481
B	252	LEU	-	expression tag	UNP O00481
B	253	ARG	-	expression tag	UNP O00481
B	254	GLN	-	expression tag	UNP O00481
B	255	ARG	-	expression tag	UNP O00481
B	256	VAL	-	expression tag	UNP O00481
B	257	GLN	-	expression tag	UNP O00481
B	258	ARG	-	expression tag	UNP O00481
B	259	LEU	-	expression tag	UNP O00481
B	260	ARG	-	expression tag	UNP O00481
B	261	ASN	-	expression tag	UNP O00481
B	262	ILE	-	expression tag	UNP O00481
B	263	VAL	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	SER	-	expression tag	UNP O00481
B	265	GLN	-	expression tag	UNP O00481
B	266	TYR	-	expression tag	UNP O00481
B	267	GLU	-	expression tag	UNP O00481
B	268	THR	-	expression tag	UNP O00481
B	269	ARG	-	expression tag	UNP O00481
B	270	TYR	-	expression tag	UNP O00481
B	271	GLY	-	expression tag	UNP O00481
B	272	PRO	-	expression tag	UNP O00481
B	273	LEU	-	expression tag	UNP O00481
B	274	GLY	-	expression tag	UNP O00481
B	275	GLY	-	expression tag	UNP O00481
B	276	THR	-	expression tag	UNP O00481
B	277	LEU	-	expression tag	UNP O00481
B	278	ASN	-	expression tag	UNP O00481
B	279	ASP	-	expression tag	UNP O00481
B	280	ILE	-	expression tag	UNP O00481
B	281	PHE	-	expression tag	UNP O00481
B	282	GLU	-	expression tag	UNP O00481
B	283	ALA	-	expression tag	UNP O00481
B	284	GLN	-	expression tag	UNP O00481
B	285	LYS	-	expression tag	UNP O00481
B	286	ILE	-	expression tag	UNP O00481
B	287	GLU	-	expression tag	UNP O00481
B	288	TRP	-	expression tag	UNP O00481
B	289	HIS	-	expression tag	UNP O00481
B	290	GLU	-	expression tag	UNP O00481
B	291	ASP	-	expression tag	UNP O00481
B	292	TYR	-	expression tag	UNP O00481
B	293	LYS	-	expression tag	UNP O00481
B	294	ASP	-	expression tag	UNP O00481
B	295	ASP	-	expression tag	UNP O00481
B	296	ASP	-	expression tag	UNP O00481
B	297	ASP	-	expression tag	UNP O00481
B	298	LYS	-	expression tag	UNP O00481

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.63Å 138.93Å 336.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 5.55	Depositor
% Data completeness (in resolution range)	56.5 (47.35-5.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 5.39Å)	Xtriage
Refinement program	BUSTER 2.10.4 (3-FEB-2022)	Depositor
R, R_{free}	0.290 , 0.336	Depositor
Wilson B-factor (Å ²)	186.2	Xtriage
Anisotropy	1.111	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3305	wwPDB-VP
Average B, all atoms (Å ²)	277.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.