



Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 08:35 pm BST

PDB ID : 5BXU
Title : Human Tankyrase-2 in Complex with Macrocyclised Extended Peptide cp4n4m5
Authors : Xu, W.; Fischer, G.; Hyvonen, M.; Itzhaki, L.
Deposited on : 2015-06-09
Resolution : 1.35 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 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) : 1.13
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

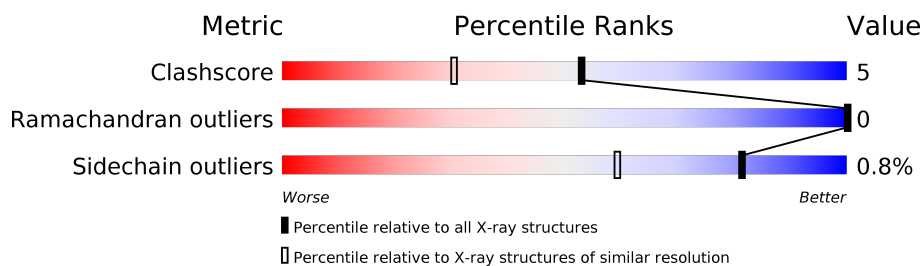
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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))
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	84% 13% ..
2	B	9	67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1576 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	1	11	0
			1334	828	245	257	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	GLY	-	expression tag	UNP Q9H2K2
A	487	SER	-	expression tag	UNP Q9H2K2

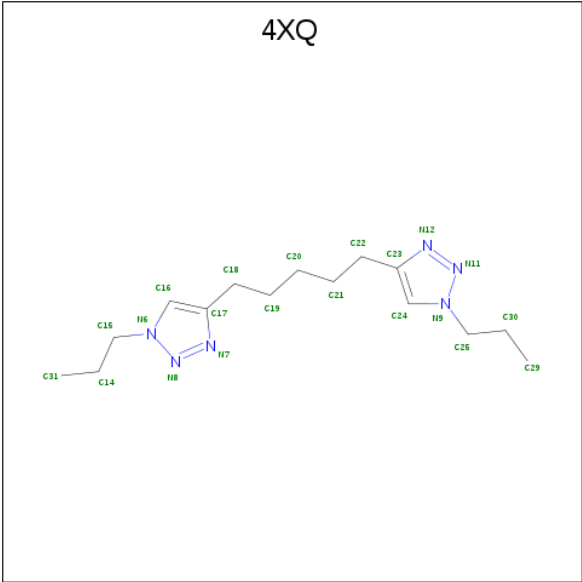
- Molecule 2 is a protein called cp4n4m5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			59	32	12	15			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 4,4'-pentane-1,5-diylbis(1-propyl-1H-1,2,3-triazole) (three-letter code: 4XQ) (formula: C₁₅H₂₆N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			21	15	6		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	5
			149	149		
5	B	12	Total	O	0	0
			12	12		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

- Molecule 1: Tankyrase-2

Chain A:  84% 13% ..



- Molecule 2: cp4n4m5

Chain B:  67% 33%



4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	31.09Å 63.28Å 72.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.90 – 1.35	Depositor
% Data completeness (in resolution range)	98.7 (28.90-1.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.156 , 0.186	Depositor
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.121	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1576	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.20% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GMA, 4XQ, ACE, CL

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	1.09	3/1358 (0.2%)	1.12	8/1838 (0.4%)
2	B	1.75	1/46 (2.2%)	1.59	1/60 (1.7%)
All	All	1.12	4/1404 (0.3%)	1.14	9/1898 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	ALA	C-N	8.16	1.47	1.33
1	A	544	TYR	CE1-CZ	-6.65	1.29	1.38
1	A	623	ARG	CD-NE	-6.26	1.35	1.46
1	A	494	ARG	CD-NE	-5.54	1.37	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	641	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	569	TYR	CB-CG-CD2	6.59	124.95	121.00
2	B	8	ALA	CB-CA-C	6.44	119.75	110.10
1	A	504	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	520[A]	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	520[B]	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	580	LYS	CD-CE-NZ	-5.39	99.30	111.70
1	A	634	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1334	0	1293	15	0
2	B	59	0	49	1	0
3	A	1	0	0	0	0
4	B	21	0	0	0	0
5	A	149	0	0	0	1
5	B	12	0	0	0	0
All	All	1576	0	1342	15	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 5.

All (15) 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:561:VAL:H	1:A:564:HIS:HD2	1.34	0.75
1:A:518:ASN:HD21	1:A:551:ASP:H	1.37	0.69
1:A:633[A]:LYS:N	1:A:633[A]:LYS:HD3	2.10	0.65
1:A:594:THR:H	1:A:597:HIS:HD2	1.43	0.64
1:A:594:THR:H	1:A:597:HIS:CD2	2.17	0.62
1:A:528:THR:H	1:A:531:HIS:HD2	1.51	0.59
1:A:528:THR:H	1:A:531:HIS:CD2	2.23	0.56
1:A:531:HIS:HE1	1:A:560:LEU:O	1.89	0.55
1:A:518:ASN:ND2	1:A:551:ASP:H	2.05	0.52
1:A:604:LYS:HZ1	2:B:9:GMA:CD	2.23	0.52
1:A:564:HIS:HE1	1:A:593:PHE:O	1.94	0.51
1:A:544:TYR:O	1:A:548:HIS:HD2	1.98	0.47
1:A:597:HIS:HE1	1:A:626:ASN:O	1.99	0.46
1:A:588:ALA:HB1	1:A:592:LYS:HA	1.99	0.45
1:A:561:VAL:H	1:A:564:HIS:CD2	2.24	0.42

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)
5:A:862:HOH:O	5:A:934:HOH:O[2_455]	1.68	0.52

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	172/164 (105%)	172 (100%)	0	0	100	100
2	B	7/9 (78%)	7 (100%)	0	0	100	100
All	All	179/173 (104%)	179 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	139/131 (106%)	137 (99%)	2 (1%)	67	36
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	142/134 (106%)	140 (99%)	2 (1%)	81	36

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	633[A]	LYS
1	A	633[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
1	A	531	HIS
1	A	548	HIS
1	A	564	HIS
1	A	597	HIS
1	A	640	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GMA	B	9	2	6,9,9	1.48	1 (16%)	7,11,11	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GMA	B	9	2	-	0/7/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	GMA	C-N2	-2.87	1.25	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9	GMA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	4XQ	B	101	2	22,22,22	2.25	6 (27%)	17,27,27	1.29	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4XQ	B	101	2	-	6/14/14/14	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	101	4XQ	C17-N7	5.69	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	101	4XQ	C16-N6	4.58	1.40	1.35
4	B	101	4XQ	C22-C23	-4.52	1.41	1.51
4	B	101	4XQ	N7-N8	-3.38	1.28	1.34
4	B	101	4XQ	N12-N11	-2.26	1.30	1.34
4	B	101	4XQ	C16-C17	2.01	1.39	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	101	4XQ	C24-C23-N12	-3.15	106.67	111.34
4	B	101	4XQ	C16-C17-N7	-2.94	106.97	111.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	101	4XQ	C20-C21-C22-C23
4	B	101	4XQ	C21-C22-C23-N12
4	B	101	4XQ	C19-C20-C21-C22
4	B	101	4XQ	C14-C15-N6-N8
4	B	101	4XQ	C30-C25-N9-C24
4	B	101	4XQ	C18-C19-C20-C21

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.