

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 6YGN

Title: Titin kinase and its flanking domains

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Deposited on : 2020-03-27

Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.23.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

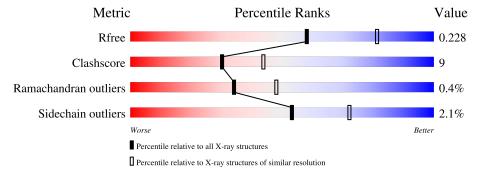
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Mol	Chain	Length	Quality of chain		
1	A	549	81%	18%	- :
1	В	549	81%	18%	_ ,



2 Entry composition (i)

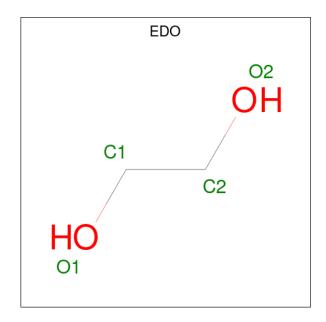
There are 4 unique types of molecules in this entry. The entry contains 9213 atoms, of which 28 are hydrogens and 0 are deuteriums.

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 Titin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	549	Total	С	N	О	S	0	0	0
1	Λ	049	4426	2800	759	849	18	0	U	0
1	B	549	Total	С	N	О	S	0	0	0
1	Ъ	949	4426	2800	759	849	18			U

• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 10				0	0
2	В	1	Total 10	C 2		O 2	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Λ	1	Total C H O		0	0			
3	A	1	14	3	8	3	0		
2	D	1	Total	С	Н	О	0	0	
3	Б	1	14	3	8	3		0	

• Molecule 4 is water.

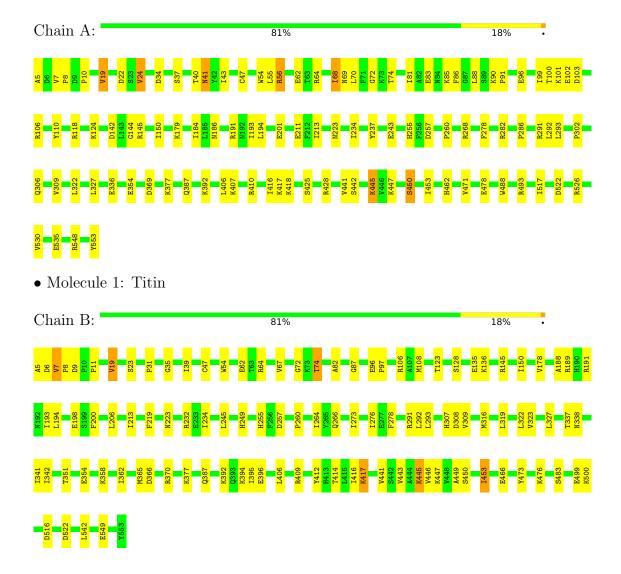
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	В	136	Total O 136 136	0	0



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. 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.

• Molecule 1: Titin





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	63.64Å 184.73Å 66.11Å	Domositon	
a, b, c, α , β , γ	90.00° 116.60° 90.00°	Depositor	
Resolution (Å)	29.82 - 2.40	Depositor	
Resolution (A)	29.82 - 2.40	EDS	
% Data completeness	98.3 (29.82-2.40)	Depositor	
(in resolution range)	98.3 (29.82-2.40)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.80 (at 2.39Å)	Xtriage	
Refinement program	PHENIX 1.13_2998	Depositor	
D D	0.172 , 0.228	Depositor	
R, R_{free}	0.172 , 0.228	DCC	
R_{free} test set	2661 reflections (5.09%)	wwPDB-VP	
Wilson B-factor (Å ²)	38.5	Xtriage	
Anisotropy	0.146	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS	
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	9213	wwPDB-VP	
Average B, all atoms (Å ²)	46.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: EDO, GOL

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.45	0/4512	0.60	1/6093~(0.0%)	
1	В	0.41	0/4512	0.58	0/6093	
All	All	0.43	0/9024	0.59	1/12186 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	A	237	TYR	CA-CB-CG	5.02	122.93	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4426	0	4391	83	1
1	В	4426	0	4391	82	0
2	A	4	6	6	0	0
2	В	4	6	6	0	0
3	A	6	8	8	0	0
3	В	6	8	8	0	0
4	A	177	0	0	8	1
4	В	136	0	0	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9185	28	8810	165	2

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 9.

The worst 5 of 165 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:291:ARG:HH21	1:B:443:VAL:HG11	1.31	0.94
1:B:266:GLN:OE1	4:B:701:HOH:O	1.84	0.93
1:B:191:ARG:NH1	4:B:704:HOH:O	2.03	0.92
1:A:377:LYS:HD2	1:A:453:ILE:HD11	1.49	0.92
1:B:245:LEU:HD13	1:B:316:MET:HE1	1.53	0.91

All (2) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
4:A:767:HOH:O	4:B:834:HOH:O[1_455]	1.99	0.21	
1:A:336:GLU:OE2	1:A:493:ARG:NH2[1_556]	2.19	0.01	

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	Perce	ntiles
1	A	547/549 (100%)	532 (97%)	13 (2%)	2 (0%)	34	48
1	В	547/549 (100%)	528 (96%)	17 (3%)	2 (0%)	34	48
All	All	1094/1098 (100%)	1060 (97%)	30 (3%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	417	LYS
1	A	223	ASN
1	В	19	VAL
1	A	19	VAL

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	Analysed Rotameric Outliers		Percentiles		
1	A	489/489 (100%)	478 (98%)	11 (2%)	52	71	
1	В	489/489 (100%)	479 (98%)	10 (2%)	55	74	
All	All	978/978 (100%)	957 (98%)	21 (2%)	53	72	

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain Res		Type
1	В	406	LEU
1	В	453	ILE
1	В	549	GLU
1	В	466	GLU
1	В	450	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	249	HIS

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are 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		Des	Link	В	ond leng	gths	В	ond ang	gles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
2	EDO	A	601	-	3,3,3	0.43	0	2,2,2	0.75	0		
3	GOL	A	602	-	5,5,5	0.34	0	5,5,5	0.46	0		
2	EDO	В	601	-	3,3,3	0.49	0	2,2,2	0.33	0		
3	GOL	В	602	-	5,5,5	0.28	0	5,5,5	0.47	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.

	\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
	2	EDO	A	601	-	-	0/1/1/1	-
	3	GOL	A	602	-	-	2/4/4/4	-
ſ	2	EDO	В	601	-	-	0/1/1/1	-
	3	GOL	В	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-O2



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

