wwPDB X-ray Structure Validation Summary Report (i)

Feb 14, 2017 – 01:21 am GMT

PDB ID	:	5EJC
Title	:	Crystal structural of the TSC1-TBC1D7 complex
Authors	:	Wang, Z.; Qin, J.; Gong, W.; Xu, W.
Deposited on	:	2015-11-01
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/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:

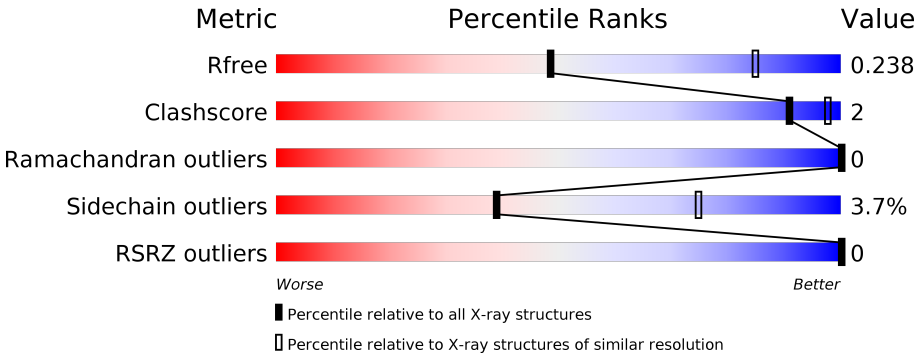
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	92%
1	B	276	91% 5%
2	C	55	45% 11% 44%
2	D	55	49% 11% 38%
2	E	55	47% 7% 42%
2	F	55	60% 11% 29%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5467 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 TBC1 domain family member 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	Se	0	0	0
			2179	1410	365	389	7	8			
1	B	267	Total	C	N	O	S	Se	0	0	0
			2169	1403	364	387	7	8			

- Molecule 2 is a protein called Hamartin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	31	Total	C	N	O	0	0	0
			256	162	45	49			
2	D	34	Total	C	N	O	0	0	0
			278	175	49	54			
2	E	32	Total	C	N	O	0	0	0
			265	167	46	52			
2	F	39	Total	C	N	O	0	0	0
			320	203	56	61			

There are 4 discrepancies between the modelled and reference sequences:

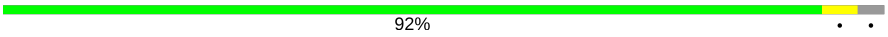
Chain	Residue	Modelled	Actual	Comment	Reference
C	938	GLY	-	expression tag	UNP Q92574
D	938	GLY	-	expression tag	UNP Q92574
E	938	GLY	-	expression tag	UNP Q92574
F	938	GLY	-	expression tag	UNP Q92574

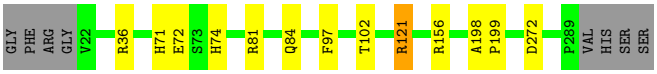
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: TBC1 domain family member 7

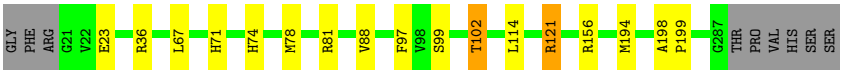
Chain A:





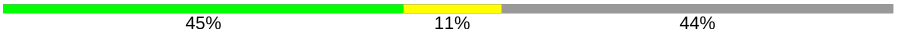
• Molecule 1: TBC1 domain family member 7

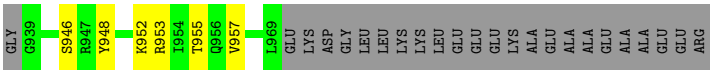
Chain B:



• Molecule 2: Hamartin

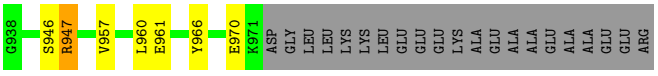
Chain C:





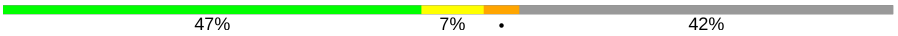
• Molecule 2: Hamartin

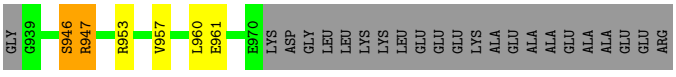
Chain D:



• Molecule 2: Hamartin

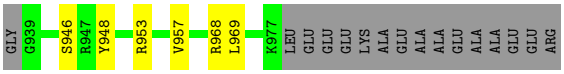
Chain E:





• Molecule 2: Hamartin

Chain F:


GLY
G939
S946
R947
Y948
R953
V957
R968
L969
K977
LEU
GLU
GLU
GLU
LYS
ALA
GLU
ALA
ALA
GLU
ALA
ALA
GLU
GLU
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	183.40Å 66.70Å 98.37Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 45.05 – 3.07	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-3.10) 94.0 (45.05-3.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.239 0.220 , 0.238	Depositor DCC
R_{free} test set	1094 reflections (5.45%)	DCC
Wilson B-factor (Å^2)	82.8	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5467	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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	0.30	0/2224	0.48	0/2998
1	B	0.29	0/2213	0.49	1/2981 (0.0%)
2	C	0.44	0/258	0.66	0/345
2	D	0.43	0/280	0.78	2/373 (0.5%)
2	E	0.43	0/267	0.90	2/357 (0.6%)
2	F	0.40	0/322	0.76	1/428 (0.2%)
All	All	0.32	0/5564	0.56	6/7482 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	947	ARG	CG-CD-NE	6.85	126.19	111.80
2	F	968	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	E	947	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	D	960	LEU	CB-CG-CD1	5.51	120.37	111.00
1	B	194	MSE	CB-CA-C	5.25	120.90	110.40

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	2179	0	2221	6	0
1	B	2169	0	2210	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	256	0	257	2	0
2	D	278	0	279	5	0
2	E	265	0	263	5	0
2	F	320	0	331	3	0
All	All	5467	0	5561	22	0

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 2.

The worst 5 of 22 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:B:114:LEU:HD12	2:D:957:VAL:HG11	1.78	0.64
2:E:947:ARG:NH2	2:F:948:TYR:CD2	2.73	0.57
1:A:71:HIS:HA	1:A:74:HIS:CD2	2.42	0.55
1:B:121:ARG:O	1:B:121:ARG:NE	2.40	0.55
1:B:71:HIS:HA	1:B:74:HIS:CD2	2.41	0.55

There are no symmetry-related clashes.

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	266/276 (96%)	256 (96%)	10 (4%)	0	100	100
1	B	265/276 (96%)	255 (96%)	10 (4%)	0	100	100
2	C	29/55 (53%)	29 (100%)	0	0	100	100
2	D	32/55 (58%)	32 (100%)	0	0	100	100
2	E	30/55 (54%)	30 (100%)	0	0	100	100
2	F	37/55 (67%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	659/772 (85%)	639 (97%)	20 (3%)	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	245/243 (101%)	237 (97%)	8 (3%)	43 77
1	B	243/243 (100%)	236 (97%)	7 (3%)	48 80
2	C	26/43 (60%)	23 (88%)	3 (12%)	6 27
2	D	28/43 (65%)	27 (96%)	1 (4%)	40 75
2	E	27/43 (63%)	25 (93%)	2 (7%)	16 49
2	F	33/43 (77%)	32 (97%)	1 (3%)	46 79
All	All	602/658 (92%)	580 (96%)	22 (4%)	39 75

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	ARG
1	B	102	THR
2	E	960	LEU
1	B	81	ARG
1	B	97	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
2	E	940	GLN
2	F	940	GLN

5.3.3 RNA

There are no RNA molecules 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, 95^{th} 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	260/276 (94%)	-0.39	0	100	100	68, 96, 125, 183	0
1	B	259/276 (93%)	-0.37	0	100	100	68, 96, 129, 147	0
2	C	31/55 (56%)	-0.28	0	100	100	85, 102, 129, 144	0
2	D	34/55 (61%)	-0.23	0	100	100	76, 100, 152, 162	0
2	E	32/55 (58%)	-0.31	0	100	100	74, 95, 130, 134	0
2	F	39/55 (70%)	-0.18	0	100	100	78, 101, 155, 162	0
All	All	655/772 (84%)	-0.35	0	100	100	68, 96, 132, 183	0

There are no RSRZ outliers to report.

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.