Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	3TVT
Title	:	Structural basis for Discs Large interaction with Pins
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Deposited on	:	2011-09-20
Resolution	:	1.60 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
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:

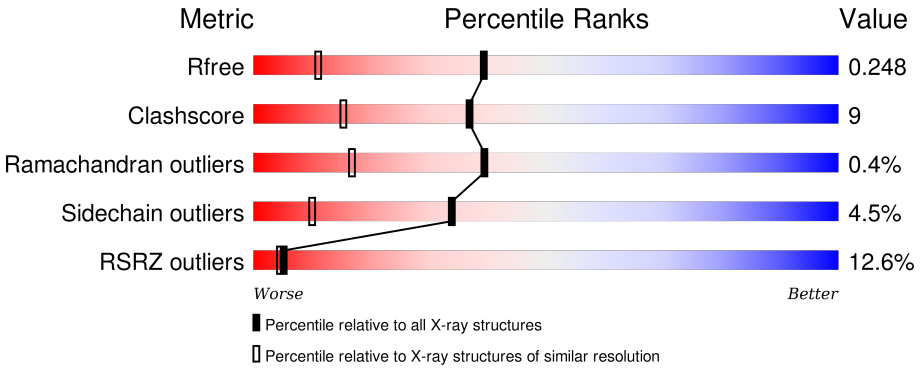
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.60 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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	292	11% 70% 15% 13%
2	B	50	6% 22% 72%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2434 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 Disks large 1 tumor suppressor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2083	1319	367	388	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	976	GLY	-	EXPRESSION TAG	UNP P31007
A	977	SER	-	EXPRESSION TAG	UNP P31007

- Molecule 2 is a protein called Partner of Inscuteable.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			117	73	20	23	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	436	ASP	SER	ENGINEERED MUTATION	UNP Q9NH88

- Molecule 3 is water.

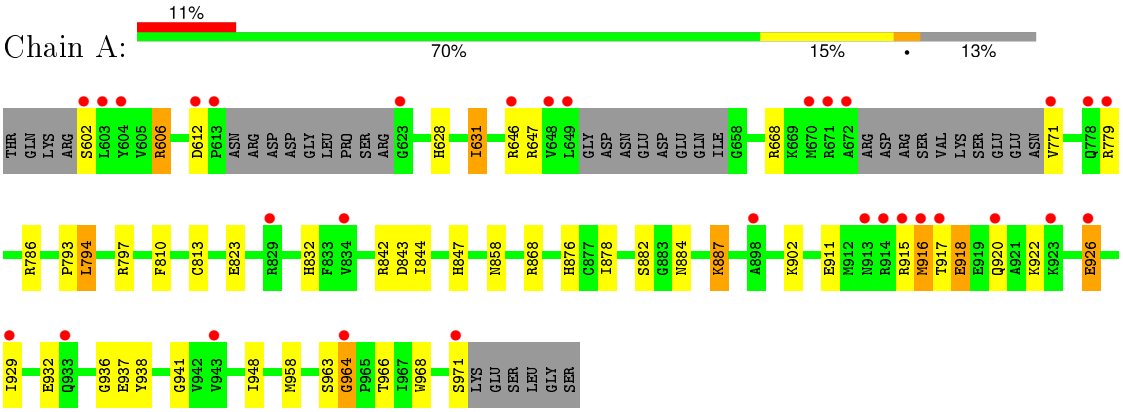
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	226	Total	O	0	0
			226	226		
3	B	8	Total	O	0	0
			8	8		

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 errors 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.

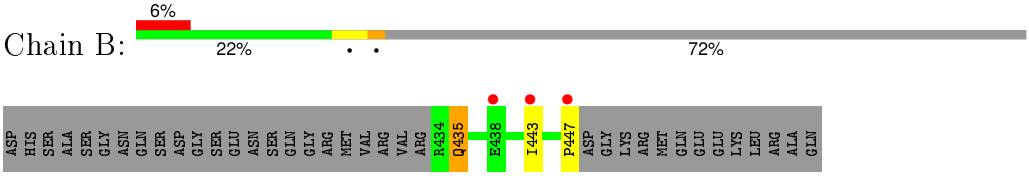
- Molecule 1: Disks large 1 tumor suppressor protein

Chain A:



- Molecule 2: Partner of Inscuteable

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	91.60Å 94.55Å 83.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.34 – 1.60 31.34 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (31.34-1.60) 99.1 (31.34-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.245 0.227 , 0.248	Depositor DCC
R_{free} test set	2400 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 50.3	EDS
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 47538 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2434	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.84	3/2128 (0.1%)	0.97	10/2872 (0.3%)
2	B	0.57	0/117	0.96	0/156
All	All	0.82	3/2245 (0.1%)	0.97	10/3028 (0.3%)

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	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	813	CYS	CB-SG	-9.00	1.67	1.82
1	A	868	ARG	CZ-NH1	5.82	1.40	1.33
1	A	964	GLY	N-CA	5.73	1.54	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	868	ARG	NE-CZ-NH1	14.19	127.39	120.30
1	A	868	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	A	668	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	668	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	823	GLU	C-N-CA	-7.52	102.90	121.70
1	A	606	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	606	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	843	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	963	SER	C-N-CA	-5.58	110.59	122.30
1	A	823	GLU	O-C-N	-5.18	114.42	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	602	SER	Peptide
1	A	964	GLY	Peptide

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	2083	0	2053	40	0
2	B	117	0	122	3	0
3	A	226	0	0	11	0
3	B	8	0	0	0	0
All	All	2434	0	2175	41	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 9.

All (41) 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:966:THR:HG23	3:A:161:HOH:O	1.37	1.17
1:A:971:SER:HB2	3:A:170:HOH:O	1.53	1.06
1:A:926:GLU:O	1:A:929:ILE:HG13	1.85	0.76
1:A:902:LYS:HE2	1:A:932:GLU:OE1	1.85	0.75
1:A:646:ARG:O	1:A:647:ARG:HB3	1.87	0.74
1:A:794:LEU:HD22	1:A:948:ILE:HD11	1.70	0.74
1:A:847:HIS:NE2	2:B:447:PRO:HD3	2.07	0.70
1:A:844:ILE:HD13	2:B:443:ILE:HD11	1.81	0.63
1:A:771:VAL:N	3:A:105:HOH:O	2.32	0.62
1:A:884:ASN:ND2	3:A:236:HOH:O	2.34	0.60
1:A:917:THR:OG1	1:A:920:GLN:HG2	2.01	0.60
1:A:779:ARG:HD3	1:A:968:TRP:CH2	2.37	0.60
1:A:786:ARG:O	1:A:876:HIS:HD2	1.85	0.58
1:A:606:ARG:NH1	1:A:631:ILE:HD11	2.18	0.58
1:A:882:SER:OG	3:A:236:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:GLU:O	1:A:918:GLU:CG	2.56	0.53
1:A:876:HIS:HE1	3:A:57:HOH:O	1.91	0.53
1:A:918:GLU:O	1:A:918:GLU:OE1	2.26	0.52
1:A:832:HIS:HE1	3:A:142:HOH:O	1.94	0.50
1:A:858:ASN:OD1	3:A:146:HOH:O	2.19	0.50
1:A:971:SER:CB	3:A:170:HOH:O	2.31	0.49
1:A:918:GLU:O	1:A:918:GLU:HG3	2.11	0.49
1:A:810:PHE:CD2	1:A:878:ILE:HG12	2.50	0.47
1:A:887:LYS:HD3	1:A:887:LYS:HA	1.78	0.46
1:A:832:HIS:HD2	3:A:10:HOH:O	1.97	0.46
1:A:793:PRO:O	1:A:794:LEU:HB2	2.15	0.46
1:A:926:GLU:O	1:A:929:ILE:CG1	2.61	0.46
1:A:916:MET:HB3	1:A:920:GLN:HB2	1.97	0.45
1:A:902:LYS:HE3	3:A:222:HOH:O	2.17	0.45
1:A:797:ARG:NH2	1:A:948:ILE:HG13	2.32	0.44
1:A:779:ARG:HD3	1:A:968:TRP:CZ2	2.53	0.44
1:A:926:GLU:HA	1:A:929:ILE:HG12	2.00	0.44
1:A:628:HIS:HE1	1:A:936:GLY:O	2.02	0.42
1:A:646:ARG:O	1:A:647:ARG:CB	2.62	0.42
1:A:941:GLY:HA3	1:A:958:MET:SD	2.58	0.42
1:A:631:ILE:CD1	1:A:631:ILE:N	2.83	0.42
1:A:937:GLU:HG2	1:A:938:TYR:CD2	2.54	0.41
1:A:902:LYS:CE	1:A:932:GLU:OE1	2.64	0.41
1:A:794:LEU:CD2	1:A:948:ILE:HD11	2.45	0.41
1:A:631:ILE:N	1:A:631:ILE:HD12	2.34	0.41
2:B:435:GLN:HG2	2:B:435:GLN:H	1.68	0.41

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	247/292 (85%)	238 (96%)	8 (3%)	1 (0%)	39 17
2	B	12/50 (24%)	12 (100%)	0	0	100 100
All	All	259/342 (76%)	250 (96%)	8 (3%)	1 (0%)	39 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	794	LEU

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	228/262 (87%)	218 (96%)	10 (4%)	35 10
2	B	14/44 (32%)	13 (93%)	1 (7%)	18 3
All	All	242/306 (79%)	231 (96%)	11 (4%)	34 10

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	612	ASP
1	A	631	ILE
1	A	842	ARG
1	A	887	LYS
1	A	911	GLU
1	A	915	ARG
1	A	916	MET
1	A	918	GLU
1	A	922	LYS
1	A	926	GLU
2	B	435	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	628	HIS
1	A	832	HIS
1	A	839	GLN
1	A	858	ASN
1	A	876	HIS
1	A	920	GLN
1	A	933	GLN
1	A	944	GLN
2	B	435	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	255/292 (87%)	0.70	31 (12%) 5 5	14, 27, 51, 67	0
2	B	14/50 (28%)	1.13	3 (21%) 1 1	28, 41, 68, 77	0
All	All	269/342 (78%)	0.72	34 (12%) 5 4	14, 28, 54, 77	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	602	SER	5.6
1	A	915	ARG	5.6
2	B	447	PRO	5.3
1	A	914	ARG	4.7
1	A	646	ARG	4.3
1	A	648	VAL	4.2
1	A	964	GLY	4.1
1	A	771	VAL	4.1
1	A	672	ALA	4.1
1	A	920	GLN	3.7
1	A	613	PRO	3.6
1	A	612	ASP	3.6
1	A	917	THR	3.5
1	A	671	ARG	3.5
1	A	603	LEU	2.8
1	A	913	ASN	2.8
1	A	929	ILE	2.7
2	B	443	ILE	2.6
1	A	778	GLN	2.6
1	A	604	TYR	2.4
1	A	834	VAL	2.4
1	A	916	MET	2.4
1	A	779	ARG	2.4
1	A	923	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	933	GLN	2.3
1	A	926	GLU	2.3
1	A	971	SER	2.3
2	B	438	GLU	2.2
1	A	898	ALA	2.2
1	A	943	VAL	2.2
1	A	649	LEU	2.1
1	A	670	MET	2.1
1	A	829	ARG	2.1
1	A	623	GLY	2.1

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.