W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:26 PM GMT

PDB ID	:	1TP3
Title	:	PDZ3 domain of PSD-95 protein complexed with KKETPV peptide ligand
Authors	:	Saro, D.; Martin, P.; Vickrey, J.F.; Griffin, A.; Kovari, L.C.; Spaller, M.R.
Deposited on	:	2004-06-15
Resolution	:	1.99 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

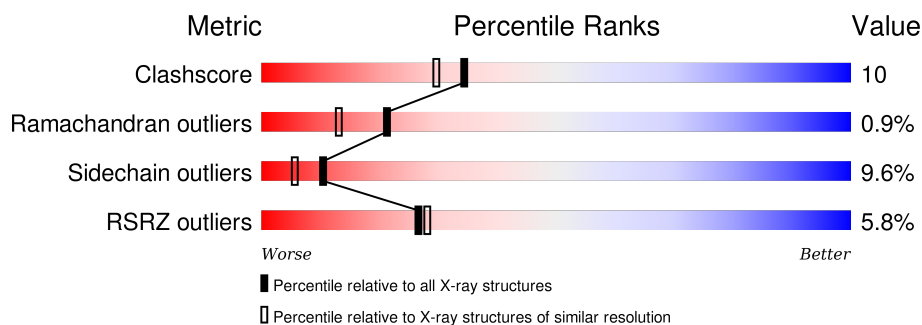|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.99 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0.9%
Sidechain outliers		9.6%
RSRZ outliers		5.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	119	4% / 63% 28% 5% · ·
2	B	6	33% / 33% 33% 17% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 974 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 Presynaptic density protein 95.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	0	0	0
			863	533	158	172			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLY	-	CLONING ARTIFACT	UNP P31016
A	298	SER	-	CLONING ARTIFACT	UNP P31016
A	299	PRO	-	CLONING ARTIFACT	UNP P31016
A	300	GLU	-	CLONING ARTIFACT	UNP P31016
A	301	PHE	-	CLONING ARTIFACT	UNP P31016
A	403	ASN	-	CLONING ARTIFACT	UNP P31016
A	404	SER	-	CLONING ARTIFACT	UNP P31016
A	405	ARG	-	CLONING ARTIFACT	UNP P31016
A	406	VAL	-	CLONING ARTIFACT	UNP P31016
A	407	ASP	-	CLONING ARTIFACT	UNP P31016
A	408	SER	-	CLONING ARTIFACT	UNP P31016
A	409	SER	-	CLONING ARTIFACT	UNP P31016
A	410	GLY	-	CLONING ARTIFACT	UNP P31016
A	411	ARG	-	CLONING ARTIFACT	UNP P31016
A	412	ILE	-	CLONING ARTIFACT	UNP P31016
A	413	VAL	-	CLONING ARTIFACT	UNP P31016
A	414	THR	-	CLONING ARTIFACT	UNP P31016
A	415	ASP	-	CLONING ARTIFACT	UNP P31016

- Molecule 2 is a protein called KKETPV peptide ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			45	28	7	10			

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total 65	O 65	0	0
3	B	1	Total 1	O 1	0	0

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: Presynaptic density protein 95
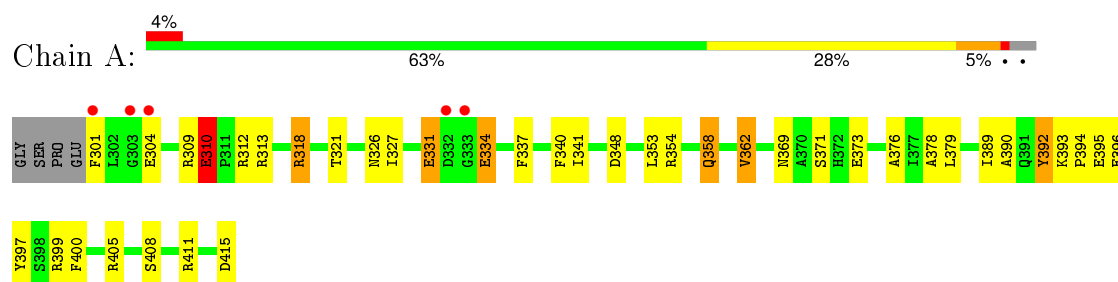
• Molecule 2: KKETPV peptide ligand
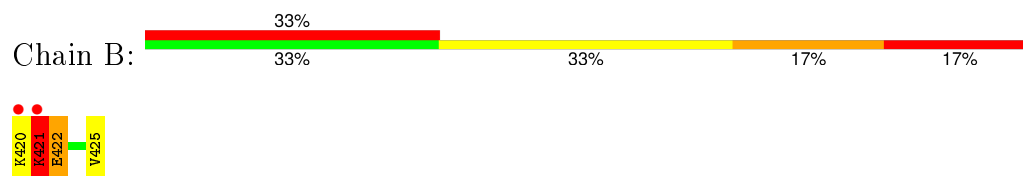
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	89.66Å 89.66Å 89.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.57 – 1.99 23.96 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.57-1.99) 99.8 (23.96-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.06 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.225 , 0.296 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Outliers	1 of 8916 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	974	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	1.86	21/874 (2.4%)	1.46	11/1177 (0.9%)
2	B	1.95	0/45	1.82	1/59 (1.7%)
All	All	1.86	21/919 (2.3%)	1.48	12/1236 (1.0%)

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
2	B	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	GLU	CD-OE1	10.93	1.37	1.25
1	A	310	GLU	CD-OE2	9.21	1.35	1.25
1	A	395	GLU	CD-OE1	8.05	1.34	1.25
1	A	396	GLU	CD-OE1	7.84	1.34	1.25
1	A	397	TYR	CG-CD2	-7.35	1.29	1.39
1	A	310	GLU	CG-CD	6.96	1.62	1.51
1	A	373	GLU	CD-OE2	6.95	1.33	1.25
1	A	358	GLN	CG-CD	6.74	1.66	1.51
1	A	395	GLU	CD-OE2	6.40	1.32	1.25
1	A	331	GLU	CD-OE2	5.95	1.32	1.25
1	A	310	GLU	CD-OE1	5.83	1.32	1.25
1	A	378	ALA	CA-CB	5.75	1.64	1.52
1	A	371	SER	CA-CB	5.55	1.61	1.52
1	A	304	GLU	CG-CD	5.48	1.60	1.51
1	A	369	ASN	C-O	-5.40	1.13	1.23
1	A	362	VAL	CB-CG1	-5.22	1.41	1.52
1	A	392	TYR	CB-CG	-5.16	1.44	1.51
1	A	373	GLU	CG-CD	5.07	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	PHE	N-CA	5.07	1.56	1.46
1	A	393	LYS	CD-CE	5.02	1.63	1.51
1	A	340	PHE	CE1-CZ	5.02	1.46	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	411	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	405	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	353	LEU	CB-CG-CD1	-7.48	98.29	111.00
2	B	421	LYS	N-CA-C	7.45	131.12	111.00
1	A	309	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	411	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	348	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	399	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	415	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	405	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	354	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	362	VAL	CG1-CB-CG2	-5.06	102.81	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	420	LYS	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	863	0	847	14	0
2	B	45	0	43	7	1
3	A	65	0	0	5	0
3	B	1	0	0	0	0
All	All	974	0	890	18	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 10.

All (18) 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)
2:B:421:LYS:HB3	2:B:421:LYS:NZ	1.84	0.93
2:B:421:LYS:HB3	2:B:421:LYS:HZ3	1.57	0.68
2:B:421:LYS:CB	2:B:421:LYS:NZ	2.61	0.62
1:A:326:ASN:ND2	2:B:422:GLU:OE1	2.33	0.61
1:A:334:GLU:CG	3:A:63:HOH:O	2.49	0.60
1:A:379:LEU:HD13	2:B:425:VAL:HG21	1.84	0.59
1:A:334:GLU:OE2	3:A:63:HOH:O	2.16	0.59
1:A:334:GLU:HG2	3:A:63:HOH:O	2.02	0.58
2:B:421:LYS:HB3	2:B:421:LYS:HZ2	1.67	0.55
1:A:376:ALA:HB3	3:A:24:HOH:O	2.08	0.52
1:A:327:ILE:O	2:B:422:GLU:HA	2.11	0.50
1:A:392:TYR:CD2	1:A:394:PRO:HD3	2.48	0.48
1:A:310:GLU:HB3	3:A:21:HOH:O	2.14	0.47
1:A:358:GLN:O	1:A:390:ALA:HA	2.15	0.46
1:A:334:GLU:HG2	1:A:400:PHE:HZ	1.84	0.41
1:A:327:ILE:HA	1:A:337:PHE:O	2.20	0.41
1:A:313:ARG:HA	1:A:389:ILE:HD13	2.03	0.40
1:A:318:ARG:HD3	1:A:321:THR:O	2.21	0.40

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)
2:B:422:GLU:OE1	2:B:422:GLU:OE1[24_565]	1.82	0.38

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	113/119 (95%)	111 (98%)	2 (2%)	0	100	100
2	B	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
All	All	117/125 (94%)	114 (97%)	2 (2%)	1 (1%)	21	13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	421	LYS

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	89/94 (95%)	82 (92%)	7 (8%)	15	9
2	B	5/6 (83%)	3 (60%)	2 (40%)	0	0
All	All	94/100 (94%)	85 (90%)	9 (10%)	10	6

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	GLU
1	A	312	ARG
1	A	318	ARG
1	A	331	GLU
1	A	341	ILE
1	A	362	VAL
1	A	408	SER
2	B	421	LYS
2	B	422	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

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, 95th 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	115/119 (96%)	0.33	5 (4%)	39	40	16, 25, 42, 58	0
2	B	6/6 (100%)	2.40	2 (33%)	0	1	39, 49, 61, 64	0
All	All	121/125 (96%)	0.43	7 (5%)	26	28	16, 25, 49, 64	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	PHE	6.0
2	B	420	LYS	5.7
1	A	304	GLU	4.1
2	B	421	LYS	3.5
1	A	332	ASP	3.4
1	A	333	GLY	2.7
1	A	303	GLY	2.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.