



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:33 PM GMT

PDB ID : 1BE9
Title : THE THIRD PDZ DOMAIN FROM THE SYNAPTIC PROTEIN PSD-95 IN
COMPLEX WITH A C-TERMINAL PEPTIDE DERIVED FROM CRIPT.
Authors : Doyle, D.A.; Lee, A.; Lewis, J.; Kim, E.; Sheng, M.; Mackinnon, R.
Deposited on : 1998-05-20
Resolution : 1.82 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

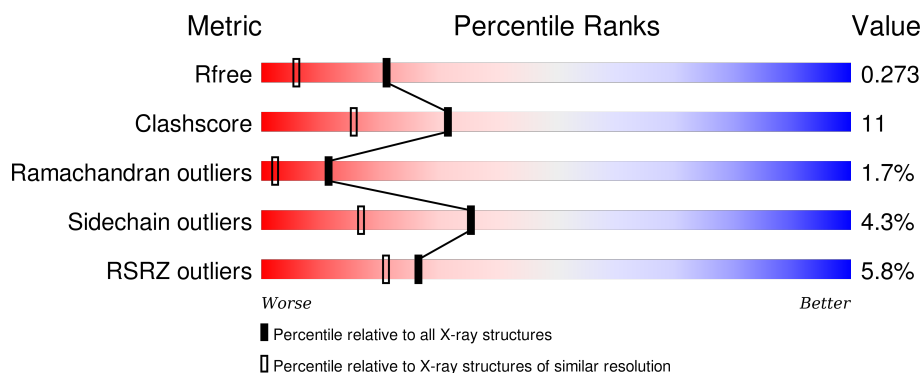
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.82 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	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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 $\leq 5\%$. 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	 6% 76% 18% . .
2	B	5	 80% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1045 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 PSD-95.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	0	0	0
			864	534	160	170			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP P31016
A	?	-	ALA	DELETION	UNP P31016
A	?	-	LYS	DELETION	UNP P31016
A	300	GLU	ASP	CONFLICT	UNP P31016
A	301	PHE	LEU	CONFLICT	UNP P31016
A	328	ILE	VAL	CONFLICT	UNP P31016
A	?	-	LYS	DELETION	UNP P31016
A	?	-	ILE	DELETION	UNP P31016
A	?	-	HIS	DELETION	UNP P31016
A	?	-	ASP	DELETION	UNP P31016
A	?	-	LEU	DELETION	UNP P31016
A	?	-	ARG	DELETION	UNP P31016
A	403	ASN	GLU	CONFLICT	UNP P31016
A	404	SER	GLN	CONFLICT	UNP P31016
A	405	ARG	LEU	CONFLICT	UNP P31016
A	406	VAL	MET	CONFLICT	UNP P31016
A	410	GLY	LEU	CONFLICT	UNP P31016
A	411	ARG	GLY	CONFLICT	UNP P31016
A	412	ILE	SER	CONFLICT	UNP P31016
A	413	VAL	GLY	CONFLICT	UNP P31016

- Molecule 2 is a protein called CRIPT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			35	20	6	9			

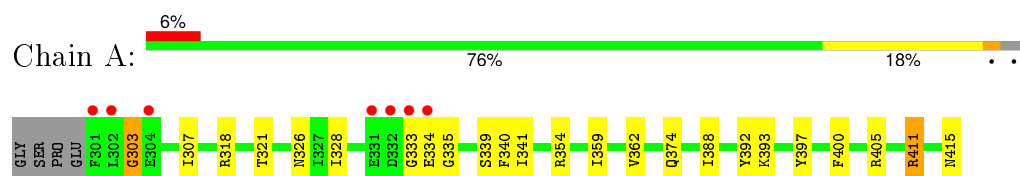
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total 137	O 137	0	0
3	B	9	Total 9	O 9	0	0

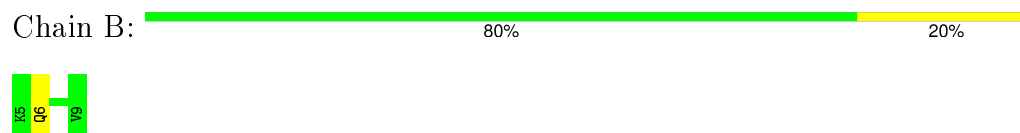
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: PSD-95



- Molecule 2: CRIPT



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	89.34Å 89.34Å 89.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.82 21.06 – 1.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.82) 96.0 (21.06-1.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.81Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.207 , 0.278 0.216 , 0.273	Depositor DCC
R_{free} test set	1088 reflections (9.84%)	DCC
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 74.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 11088 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1045	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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, 0.375 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	0.36	0/875	0.62	0/1178
2	B	0.51	0/34	0.53	0/44
All	All	0.36	0/909	0.62	0/1222

There are no bond length outliers.

There are no bond angle outliers.

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	864	0	853	19	0
2	B	35	0	30	2	0
3	A	137	0	0	2	0
3	B	9	0	0	0	0
All	All	1045	0	883	19	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 11.

All (19) 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:328:ILE:HG22	2:B:6:GLN:HG2	1.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:HH11	1:A:411:ARG:HG2	1.49	0.76
1:A:405:ARG:HE	1:A:415:ASN:HD21	1.44	0.65
1:A:393:LYS:HE2	3:A:13:HOH:O	1.99	0.61
1:A:333:GLY:O	1:A:335:GLY:N	2.38	0.57
1:A:328:ILE:HG22	2:B:6:GLN:CG	2.33	0.56
1:A:326:ASN:HB2	1:A:340:PHE:HB3	1.88	0.55
1:A:307:ILE:HD11	1:A:411:ARG:HD3	1.88	0.55
1:A:328:ILE:HD11	1:A:397:TYR:CE1	2.42	0.54
1:A:321:THR:HB	3:A:143:HOH:O	2.10	0.50
1:A:303:GLY:HA2	1:A:411:ARG:HH21	1.78	0.49
1:A:328:ILE:HD12	1:A:400:PHE:CB	2.43	0.48
1:A:362:VAL:O	1:A:362:VAL:HG13	2.13	0.48
1:A:359:ILE:HG23	1:A:388:ILE:HG23	1.97	0.46
1:A:354:ARG:HD2	1:A:392:TYR:CE1	2.52	0.44
1:A:411:ARG:NH1	1:A:411:ARG:HG2	2.22	0.44
1:A:405:ARG:NE	1:A:415:ASN:HD21	2.14	0.42
1:A:328:ILE:HD13	1:A:339:SER:HB3	2.02	0.41
1:A:328:ILE:HD12	1:A:400:PHE:CG	2.55	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	113/119 (95%)	109 (96%)	2 (2%)	2 (2%)	11	2
2	B	3/5 (60%)	3 (100%)	0	0	100	100
All	All	116/124 (94%)	112 (97%)	2 (2%)	2 (2%)	11	2

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	GLU
1	A	303	GLY

5.3.2 Protein sidechains ⓘ

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%)	85 (96%)	4 (4%)	34	15
2	B	4/5 (80%)	4 (100%)	0	100	100
All	All	93/99 (94%)	89 (96%)	4 (4%)	35	17

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	ARG
1	A	341	ILE
1	A	374	GLN
1	A	411	ARG

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

Mol	Chain	Res	Type
1	A	415	ASN

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 [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%)	0.18	7 (6%) 25 20	10, 18, 49, 56	0
2	B	5/5 (100%)	0.00	0 100 100	14, 16, 23, 32	0
All	All	120/124 (96%)	0.17	7 (5%) 26 21	10, 18, 49, 56	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	ASP	4.4
1	A	301	PHE	3.6
1	A	333	GLY	3.5
1	A	334	GLU	2.5
1	A	304	GLU	2.2
1	A	331	GLU	2.1
1	A	302	LEU	2.1

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.