

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 17, 2023 – 12:53 PM EDT

PDB ID	:	2G2L
Title	:	Crystal Structure of the Second PDZ Domain of SAP97 in Complex with a
		GluR-A C-terminal Peptide
Authors	:	Von Ossowski, I.; Oksanen, E.; Von Ossowski, L.; Cai, C.; Sundberg, M.;
		Goldman, A.; Keinanen, K.
Deposited on	:	2006-02-16
Resolution	:	2.35  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

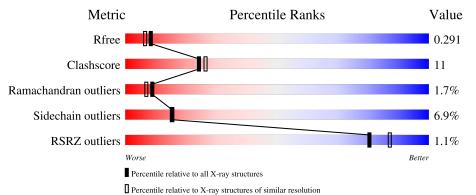
MolProbity Xtriage (Phenix) EDS	:	
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996)

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.35 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	$1164 \ (2.36-2.36)$
Clashscore	141614	1232(2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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% 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	А	105	58%	27%	•	14%			
1	В	105	<sup>2%</sup> 67%	16%	•	14%			
2	С	18	6% 17% 7	8%					
2	D	18	6% 94%						



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1366 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	90	Total	С	Ν	0	S	0	0	0
	90	657	421	111	123	2	0	0	0	
1	В	90	Total	С	Ν	0	S	0	0	0
	ГБ	90	631	402	105	122	2		0	0

• Molecule 1 is a protein called Synapse-associated protein 97.

Chain	Residue	Modelled	Actual	Comment	Reference
А	314	MET	-	initiating methionine	UNP Q62696
А	315	GLU	ARG	SEE REMARK 999	UNP Q62696
А	317	ILE	ASN	SEE REMARK 999	UNP Q62696
А	318	MET	HIS	SEE REMARK 999	UNP Q62696
А	402	VAL	ALA	SEE REMARK 999	UNP Q62696
А	411	SER	-	expression tag	UNP Q62696
А	412	ARG	-	expression tag	UNP Q62696
А	413	HIS	-	expression tag	UNP Q62696
А	414	HIS	-	expression tag	UNP Q62696
А	415	HIS	-	expression tag	UNP Q62696
А	416	HIS	-	expression tag	UNP Q62696
А	417	HIS	-	expression tag	UNP Q62696
А	418	HIS	-	expression tag	UNP Q62696
В	314	MET	-	initiating methionine	UNP Q62696
В	315	GLU	ARG	SEE REMARK 999	UNP Q62696
В	317	ILE	ASN	SEE REMARK 999	UNP Q62696
В	318	MET	HIS	SEE REMARK 999	UNP Q62696
В	402	VAL	ALA	SEE REMARK 999	UNP Q62696
В	411	SER	-	expression tag	UNP Q62696
В	412	ARG	-	expression tag	UNP Q62696
В	413	HIS	-	expression tag	UNP Q62696
В	414	HIS	-	expression tag	UNP Q62696
В	415	HIS	-	expression tag	UNP Q62696
В	416	HIS	-	expression tag	UNP Q62696
В	417	HIS	-	expression tag	UNP Q62696

There are 26 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference
В	418	HIS	-	expression tag	UNP Q62696

• Molecule 2 is a protein called 18-mer peptide from glutamate receptor, ionotropic, AMPA1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	4	Total         C         N         O           25         15         4         6	0	0	0
2	D	1	Total         C         N         O           9         6         1         2	0	0	0

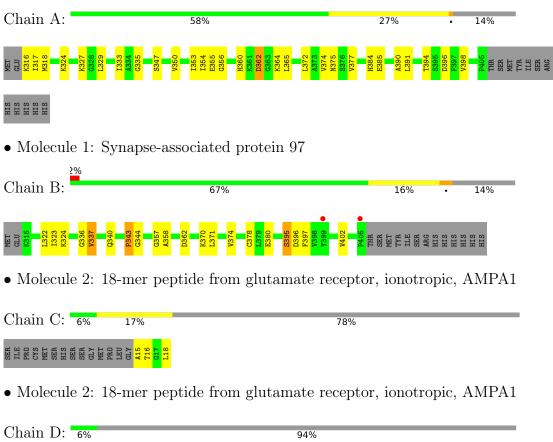
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	24	Total O 24 24	0	0
3	В	20	TotalO2020	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 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: Synapse-associated protein 97

SER TLE PRO CYS MET MET HIS SER SER SER SER MET MET MET PRO CLY CLY CLY



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	$34.76\text{\AA}$ $54.44\text{\AA}$ $55.14\text{\AA}$	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $93.95^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	38.63 - 2.35	Depositor
Resolution (A)	38.69 - 2.35	EDS
% Data completeness	100.0 (38.63 - 2.35)	Depositor
(in resolution range)	97.5(38.69-2.35)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.50 (at 2.37 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
$R, R_{free}$	0.218 , $0.295$	Depositor
It, Itfree	0.215 , $0.291$	DCC
$R_{free}$ test set	422 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.8	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, $50.0$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1366	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 10.58% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.82	0/666	0.87	0/898	
1	В	0.75	0/638	0.79	1/865~(0.1%)	
2	С	0.60	0/24	0.69	0/30	
2	D	1.09	0/8	0.94	0/8	
All	All	0.79	0/1336	0.83	1/1801~(0.1%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	322	LEU	CA-CB-CG	5.75	128.51	115.30

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	А	657	0	677	18	0
1	В	631	0	603	11	0
2	С	25	0	25	3	0
2	D	9	0	10	0	0
3	А	24	0	0	4	0
3	В	20	0	0	2	0
All	All	1366	0	1315	29	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.

The worst 5 of 29 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:356:GLY:N	1:A:360:HIS:ND1	2.25	0.82
1:A:394:THR:HA	3:A:38:HOH:O	1.81	0.79
1:B:378:CYS:SG	1:B:380:GLU:HG3	2.36	0.66
1:A:329:LEU:HD21	1:A:398:VAL:HG21	1.80	0.63
1:B:374:VAL:O	1:B:374:VAL:HG13	2.02	0.59

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	А	88/105~(84%)	78~(89%)	9 (10%)	1 (1%)	14 13
1	В	88/105~(84%)	78~(89%)	8 (9%)	2(2%)	6 4
2	С	2/18 (11%)	2 (100%)	0	0	100 100
All	All	178/228 (78%)	158 (89%)	17 (10%)	3 (2%)	9 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	355	GLU
1	В	337	VAL
1	В	343	PRO



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	69/87~(79%)	64~(93%)	5(7%)	14	14
1	В	59/87~(68%)	55~(93%)	4 (7%)	16	16
2	С	2/14 (14%)	2 (100%)	0	100	100
2	D	1/14~(7%)	1 (100%)	0	100	100
All	All	131/202~(65%)	122 (93%)	9~(7%)	15	15

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	В	370	LYS
1	В	395	SER
1	А	385	GLU
1	А	396	ASP
1	В	343	PRO

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

Mol	Chain	Res	Type
1	А	339	ASN

#### 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)

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,  $95^{th}$  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	А	90/105~(85%)	0.00	0 100 100	28, 41, 54, 56	0
1	В	90/105~(85%)	0.15	2 (2%) 62 72	27, 54, 63, 72	0
2	С	4/18~(22%)	0.64	0 100 100	60, 61, 63, 64	0
2	D	1/18~(5%)	1.99	0 100 100	64, 64, 64, 64	0
All	All	185/246~(75%)	0.10	2 (1%) 80 87	27, 48, 63, 72	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	405	PRO	5.8
1	В	399	TYR	2.0

#### 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 monosaccharides 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.

