



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:46 AM GMT

PDB ID : 4IIM  
Title : Crystal structure of the Second SH3 Domain of ITSN1 bound with a synthetic peptide  
Authors : Dong, A.; Guan, X.; Huang, H.; Wernimont, A.; Gu, J.; Sidhu, S.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Tong, Y.; Structural Genomics Consortium (SGC)  
Deposited on : 2012-12-20  
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

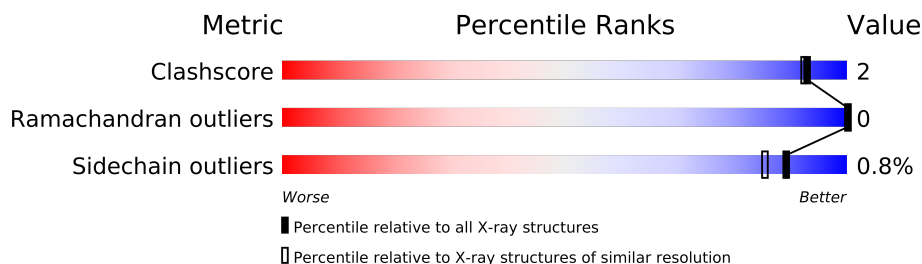
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	70	
1	B	70	
2	C	12	
2	D	12	
2	E	12	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1333 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Intersectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	3	0
			495	325	83	86	1			
1	B	55	Total	C	N	O	S	0	1	0
			467	309	78	79	1			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	904	GLY	-	EXPRESSION TAG	UNP Q15811
A	905	ALA	-	EXPRESSION TAG	UNP Q15811
A	906	ALA	-	EXPRESSION TAG	UNP Q15811
A	907	GLN	-	EXPRESSION TAG	UNP Q15811
A	908	PRO	-	EXPRESSION TAG	UNP Q15811
A	909	ALA	-	EXPRESSION TAG	UNP Q15811
A	910	MET	-	EXPRESSION TAG	UNP Q15811
A	911	ALA	-	EXPRESSION TAG	UNP Q15811
A	912	GLN	-	EXPRESSION TAG	UNP Q15811
A	913	GLY	-	EXPRESSION TAG	UNP Q15811
A	914	ALA	-	EXPRESSION TAG	UNP Q15811
A	915	LEU	-	EXPRESSION TAG	UNP Q15811
A	971	ALA	-	EXPRESSION TAG	UNP Q15811
A	972	ALA	-	EXPRESSION TAG	UNP Q15811
A	973	ALA	-	EXPRESSION TAG	UNP Q15811
B	904	GLY	-	EXPRESSION TAG	UNP Q15811
B	905	ALA	-	EXPRESSION TAG	UNP Q15811
B	906	ALA	-	EXPRESSION TAG	UNP Q15811
B	907	GLN	-	EXPRESSION TAG	UNP Q15811
B	908	PRO	-	EXPRESSION TAG	UNP Q15811
B	909	ALA	-	EXPRESSION TAG	UNP Q15811
B	910	MET	-	EXPRESSION TAG	UNP Q15811
B	911	ALA	-	EXPRESSION TAG	UNP Q15811
B	912	GLN	-	EXPRESSION TAG	UNP Q15811
B	913	GLY	-	EXPRESSION TAG	UNP Q15811

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	914	ALA	-	EXPRESSION TAG	UNP Q15811
B	915	LEU	-	EXPRESSION TAG	UNP Q15811
B	971	ALA	-	EXPRESSION TAG	UNP Q15811
B	972	ALA	-	EXPRESSION TAG	UNP Q15811
B	973	ALA	-	EXPRESSION TAG	UNP Q15811

- Molecule 2 is a protein called peptide ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total 109	C 72	N 17	O 19	S 1	0	2	0
2	D	12	Total 107	C 70	N 17	O 18	S 2	0	1	0
2	E	5	Total 41	C 28	N 6	O 6	S 1	0	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	X	0	0
			5	5		
3	A	2	Total	X	0	0
			2	2		
3	D	1	Total	X	0	0
			1	1		
3	C	3	Total	X	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	3
			50	50		
4	C	9	Total	O	0	0
			9	9		
4	B	34	Total	O	0	1
			35	35		
4	D	8	Total	O	0	0
			8	8		
4	E	1	Total	O	0	0
			1	1		

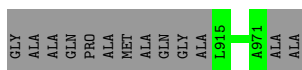
### 3 Residue-property plots

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.

Note EDS failed to run properly.

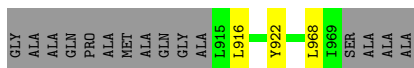
- Molecule 1: Intersectin-1

Chain A: 



- Molecule 1: Intersectin-1

Chain B: 



- Molecule 2: peptide ligand

Chain C: 



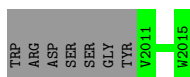
- Molecule 2: peptide ligand

Chain D: 



- Molecule 2: peptide ligand

Chain E: 



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.05Å 51.39Å 69.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.12 – 1.80	Depositor
% Data completeness (in resolution range)	95.5 (29.12-1.80)	Depositor
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0032, COOT 0.6.2	Depositor
R, $R_{free}$	0.188 , 0.243	Depositor
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.400	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 13507 reflections	Xtriage
Total number of atoms	1333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX

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	0.58	0/519	0.70	0/704
1	B	0.53	0/485	0.59	0/657
2	C	0.58	0/120	0.62	0/162
2	D	0.63	0/115	0.63	0/154
2	E	0.74	0/43	0.70	0/57
All	All	0.57	0/1282	0.64	0/1734

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	495	0	482	0	0
1	B	467	0	454	1	0
2	C	109	0	100	1	0
2	D	107	0	95	2	0
2	E	41	0	37	0	0
3	A	2	0	0	0	0
3	B	5	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	50	0	0	0	0
4	B	35	0	0	0	0
4	C	9	0	0	0	0
4	D	8	0	0	1	0
4	E	1	0	0	0	0
All	All	1333	0	1168	4	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (4) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:2003:ASP:HB2	4:D:2205:HOH:O	1.81	0.80
2:D:2005:SER:O	2:D:2009[A]:MET:HG3	2.13	0.47
2:C:2004:SER:O	2:C:2008[B]:VAL:HG22	2.20	0.42
1:B:916:LEU:HD11	1:B:968:LEU:HD22	2.00	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	58/70 (83%)	55 (95%)	3 (5%)	0	100	100
1	B	54/70 (77%)	52 (96%)	2 (4%)	0	100	100
2	C	12/12 (100%)	12 (100%)	0	0	100	100
2	D	11/12 (92%)	11 (100%)	0	0	100	100
2	E	3/12 (25%)	3 (100%)	0	0	100	100
All	All	138/176 (78%)	133 (96%)	5 (4%)	0	100	100

There are no Ramachandran outliers to report.



### 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	52/54 (96%)	52 (100%)	0	100	100
1	B	48/54 (89%)	47 (98%)	1 (2%)	66	51
2	C	12/10 (120%)	12 (100%)	0	100	100
2	D	11/10 (110%)	11 (100%)	0	100	100
2	E	4/10 (40%)	4 (100%)	0	100	100
All	All	127/138 (92%)	126 (99%)	1 (1%)	89	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	922	TYR

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

Mol	Chain	Res	Type
1	B	917	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 11 ligands modelled in this entry, 11 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.