



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:04 AM GMT

PDB ID : 2X0C  
Title : STRUCTURE OF THE TALIN ROD RESIDUES 1359-1659  
Authors : Gingras, A.R.; Goult, B.T.; Bate, N.; Barsukov, I.L.; Emsley, J.; Critchely, D.R.  
Deposited on : 2009-12-08  
Resolution : 2.00 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>

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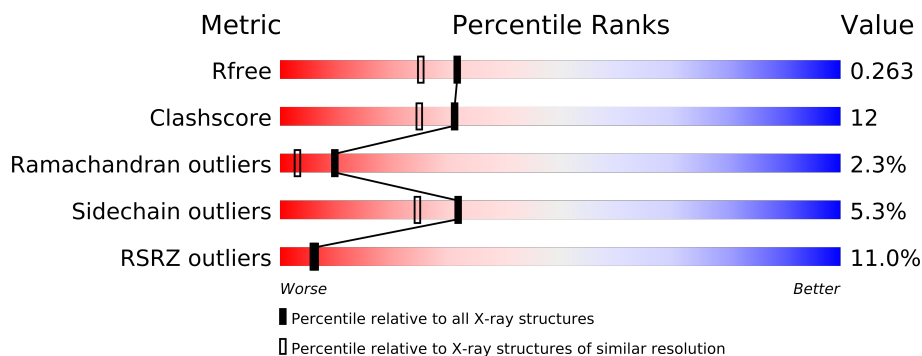
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	309	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2455 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 TALIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2270	1395	408	452	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1351	GLY	-	EXPRESSION TAG	UNP P26039
A	1352	ILE	-	EXPRESSION TAG	UNP P26039
A	1353	ASP	-	EXPRESSION TAG	UNP P26039
A	1354	PRO	-	EXPRESSION TAG	UNP P26039
A	1355	PHE	-	EXPRESSION TAG	UNP P26039
A	1356	THR	-	EXPRESSION TAG	UNP P26039
A	1357	LYS	-	EXPRESSION TAG	UNP P26039
A	1358	HIS	-	EXPRESSION TAG	UNP P26039

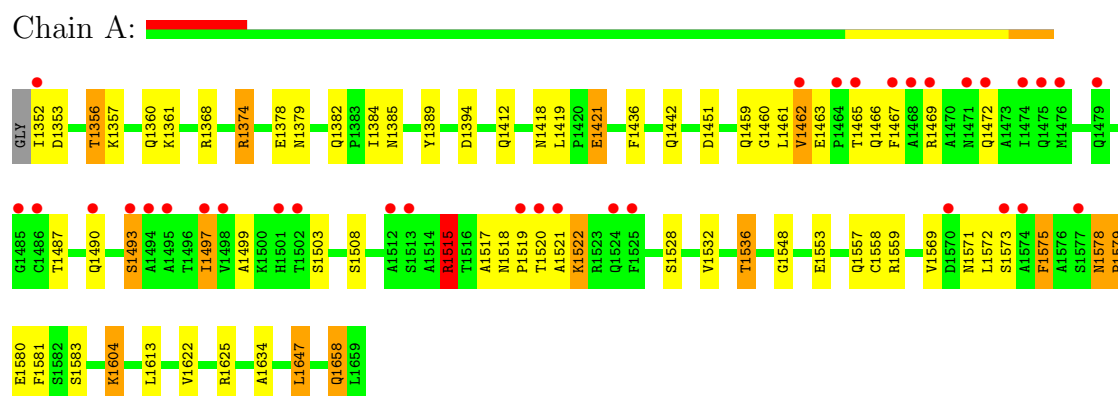
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	185	Total	O	0	0
			185	185		

### 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 ( $\text{RSRZ} > 2$ ). 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: TALIN-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.00Å 66.81Å 185.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 46.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.00) 99.6 (46.43-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.212 , 0.264 0.212 , 0.263	Depositor DCC
$R_{free}$ test set	1641 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 32820 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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

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	1.28	11/2302 (0.5%)	1.03	5/3123 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1378	GLU	CD-OE2	8.53	1.35	1.25
1	A	1622	VAL	CB-CG1	7.41	1.68	1.52
1	A	1421	GLU	CD-OE2	7.02	1.33	1.25
1	A	1558	CYS	CB-SG	-6.13	1.71	1.82
1	A	1378	GLU	CB-CG	5.98	1.63	1.52
1	A	1625	ARG	CB-CG	5.64	1.67	1.52
1	A	1436	PHE	CD2-CE2	-5.41	1.28	1.39
1	A	1378	GLU	CG-CD	5.31	1.59	1.51
1	A	1634	ALA	CA-CB	5.17	1.63	1.52
1	A	1374	ARG	CB-CG	-5.11	1.38	1.52
1	A	1421	GLU	CB-CG	5.08	1.61	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1559	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	1604	LYS	CD-CE-NZ	-5.92	98.09	111.70
1	A	1379	ASN	C-N-CD	5.72	140.41	128.40
1	A	1356	THR	OG1-CB-CG2	-5.39	97.59	110.00
1	A	1647	LEU	CA-CB-CG	5.16	127.16	115.30

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	2270	0	2265	53	0
2	A	185	0	0	10	0
All	All	2455	0	2265	53	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 12.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1532:VAL:O	1:A:1536:THR:HG22	1.42	1.17
1:A:1352:ILE:N	2:A:2017:HOH:O	1.92	1.02
1:A:1384:ILE:H	1:A:1442:GLN:NE2	1.68	0.92
1:A:1579:PRO:O	1:A:1581:PHE:N	2.14	0.81
1:A:1353:ASP:OD2	1:A:1356:THR:HG23	1.81	0.80
1:A:1360:GLN:OE1	2:A:2024:HOH:O	2.03	0.77
1:A:1352:ILE:HG13	1:A:1357:LYS:CE	2.18	0.73
1:A:1352:ILE:HG13	1:A:1357:LYS:HE2	1.71	0.73
1:A:1352:ILE:CG1	1:A:1357:LYS:HE2	2.21	0.69
1:A:1578:ASN:HB3	1:A:1579:PRO:CD	2.24	0.68
1:A:1368:ARG:NH1	2:A:2035:HOH:O	2.27	0.67
1:A:1461:LEU:HD13	1:A:1581:PHE:HD1	1.61	0.66
1:A:1461:LEU:CD1	1:A:1581:PHE:HD1	2.09	0.66
1:A:1557:GLN:NE2	2:A:2125:HOH:O	2.29	0.66
1:A:1394:ASP:OD2	2:A:2056:HOH:O	2.14	0.64
1:A:1361:LYS:NZ	2:A:2025:HOH:O	2.28	0.63
1:A:1384:ILE:H	1:A:1442:GLN:HE22	1.42	0.62
1:A:1518:ASN:OD1	1:A:1520:THR:HG22	2.00	0.61
1:A:1412:GLN:HG3	2:A:2070:HOH:O	2.00	0.61
1:A:1461:LEU:HD13	1:A:1581:PHE:CD1	2.35	0.60
1:A:1451:ASP:HB2	2:A:2099:HOH:O	2.01	0.60
1:A:1467:PHE:HB3	1:A:1573:SER:HB2	1.83	0.60
1:A:1466:GLN:HA	1:A:1469:ARG:NH1	2.19	0.58
1:A:1521:ALA:HB2	1:A:1581:PHE:HZ	1.69	0.57
1:A:1462:VAL:HG13	1:A:1508:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1384:ILE:N	1:A:1442:GLN:NE2	2.48	0.57
1:A:1463:GLU:HB2	1:A:1466:GLN:HB2	1.88	0.56
1:A:1459:GLN:O	1:A:1515:ARG:NH2	2.38	0.55
1:A:1519:PRO:HA	1:A:1522:LYS:HB3	1.89	0.55
1:A:1460:GLY:H	1:A:1583:SER:HB3	1.72	0.55
1:A:1389:TYR:CB	1:A:1658:GLN:HG2	2.38	0.53
1:A:1384:ILE:H	1:A:1442:GLN:HE21	1.48	0.53
1:A:1384:ILE:N	1:A:1442:GLN:HE22	2.07	0.52
1:A:1493:SER:O	1:A:1497:ILE:HG23	2.09	0.52
1:A:1356:THR:HG22	1:A:1419:LEU:HD11	1.92	0.52
1:A:1353:ASP:OD2	1:A:1356:THR:CG2	2.56	0.52
1:A:1352:ILE:HG13	1:A:1357:LYS:CG	2.40	0.51
1:A:1532:VAL:O	1:A:1536:THR:CG2	2.36	0.51
1:A:1418:ASN:HB3	1:A:1421:GLU:OE2	2.10	0.50
1:A:1571:ASN:O	1:A:1575:PHE:HB3	2.11	0.50
1:A:1578:ASN:HB3	1:A:1579:PRO:HD2	1.94	0.49
1:A:1374:ARG:HD3	2:A:2047:HOH:O	2.14	0.48
1:A:1459:GLN:HG3	1:A:1515:ARG:NH2	2.28	0.47
1:A:1499:ALA:O	1:A:1503:SER:HB2	2.15	0.47
1:A:1487:THR:HG23	1:A:1490:GLN:OE1	2.18	0.44
1:A:1389:TYR:HB2	1:A:1658:GLN:HG2	1.99	0.44
1:A:1385:ASN:H	1:A:1442:GLN:NE2	2.16	0.43
1:A:1613:LEU:C	1:A:1613:LEU:HD23	2.39	0.43
1:A:1352:ILE:CG1	1:A:1357:LYS:CE	2.90	0.42
1:A:1569:VAL:O	1:A:1573:SER:N	2.49	0.41
1:A:1522:LYS:HE2	1:A:1522:LYS:HB2	1.73	0.41
1:A:1382:GLN:O	1:A:1384:ILE:HD12	2.22	0.40
1:A:1604:LYS:NZ	2:A:2143:HOH:O	2.47	0.40

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	306/309 (99%)	288 (94%)	11 (4%)	7 (2%)	10   3



All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1580	GLU
1	A	1515	ARG
1	A	1517	ALA
1	A	1578	ASN
1	A	1579	PRO
1	A	1548	GLY
1	A	1462	VAL

### 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	243/243 (100%)	230 (95%)	13 (5%)	32	24

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1465	THR
1	A	1472	GLN
1	A	1493	SER
1	A	1497	ILE
1	A	1515	ARG
1	A	1522	LYS
1	A	1528	SER
1	A	1536	THR
1	A	1553	GLU
1	A	1572	LEU
1	A	1575	PHE
1	A	1647	LEU
1	A	1658	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1358	HIS
1	A	1360	GLN

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Mol	Chain	Res	Type
1	A	1442	GLN
1	A	1466	GLN
1	A	1527	GLN
1	A	1557	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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	308/309 (99%)	0.64	34 (11%) 6 6	15, 34, 68, 80	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1498	VAL	5.9
1	A	1497	ILE	5.8
1	A	1521	ALA	5.8
1	A	1467	PHE	5.6
1	A	1468	ALA	5.5
1	A	1520	THR	5.2
1	A	1465	THR	4.7
1	A	1472	GLN	4.4
1	A	1502	THR	4.3
1	A	1476	MET	3.9
1	A	1485	GLY	3.8
1	A	1474	ILE	3.6
1	A	1573	SER	3.5
1	A	1495	ALA	3.4
1	A	1479	GLN	3.2
1	A	1524	GLN	3.2
1	A	1574	ALA	3.2
1	A	1513	SER	3.1
1	A	1493	SER	3.1
1	A	1475	GLN	2.8
1	A	1464	PRO	2.7
1	A	1469	ARG	2.6
1	A	1494	ALA	2.5
1	A	1501	HIS	2.4
1	A	1352	ILE	2.3
1	A	1577	SER	2.3
1	A	1462	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1570	ASP	2.2
1	A	1490	GLN	2.2
1	A	1525	PHE	2.1
1	A	1486	CYS	2.1
1	A	1512	ALA	2.0
1	A	1519	PRO	2.0
1	A	1471	ASN	2.0

## 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.