



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:55 PM UTC

PDB ID : 2X0C / pdb_00002x0c
Title : Crystal Structure of the R7R8 domains of Talin
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

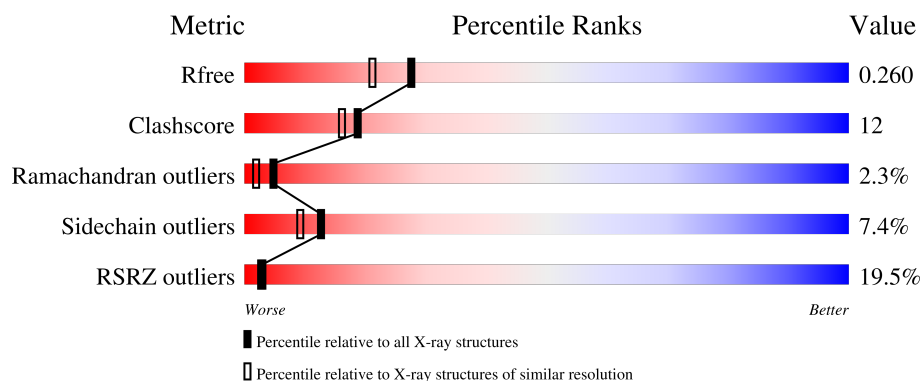
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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 $\leq 5\%$. 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	309	19% 72% 22% ..

2 Entry composition

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

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

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

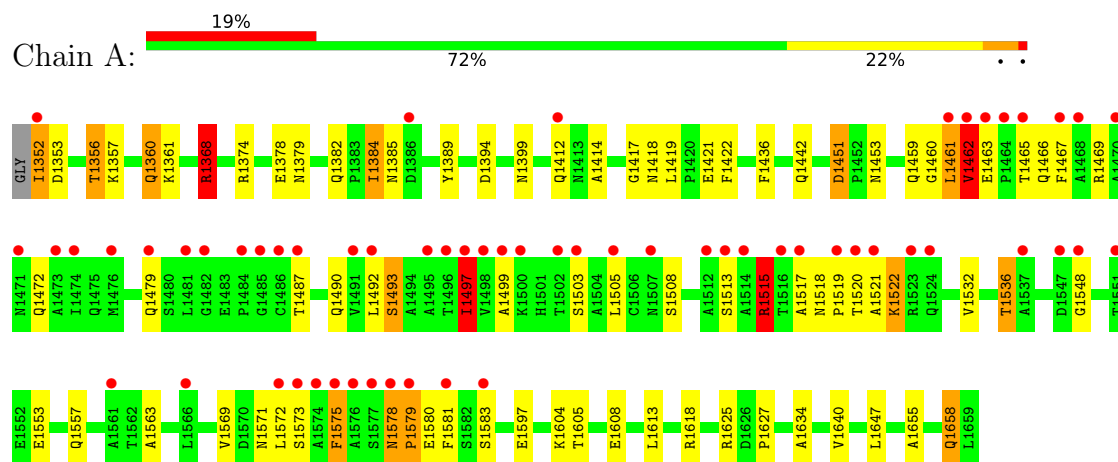
- Molecule 2 is water.

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

3 Residue-property plots [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: TALIN-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.00Å 66.81Å 185.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.00) 99.6 (50.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.212 , 0.264 0.210 , 0.260	Depositor DCC
R_{free} test set	1641 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2455	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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	1.58	16/2302 (0.7%)	1.43	15/3123 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1368	ARG	N-CA	7.57	1.55	1.46
1	A	1634	ALA	CA-CB	6.42	1.63	1.53
1	A	1563	ALA	CA-CB	6.17	1.61	1.53
1	A	1384	ILE	CA-CB	6.10	1.62	1.54
1	A	1414	ALA	CA-CB	5.74	1.62	1.53
1	A	1451	ASP	CA-C	5.74	1.59	1.53
1	A	1655	ALA	CA-C	5.74	1.59	1.52
1	A	1417	GLY	C-O	5.70	1.31	1.23
1	A	1627	PRO	CA-C	5.69	1.57	1.52
1	A	1384	ILE	CG1-CD1	5.50	1.73	1.51
1	A	1360	GLN	CD-NE2	5.42	1.44	1.33
1	A	1436	PHE	N-CA	-5.38	1.40	1.46
1	A	1618	ARG	CA-C	5.23	1.59	1.52
1	A	1422	PHE	N-CA	5.17	1.52	1.46
1	A	1625	ARG	CB-CG	5.11	1.67	1.52
1	A	1378	GLU	CD-OE2	5.10	1.35	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1379	ASN	CA-C-N	-13.48	103.65	120.23
1	A	1379	ASN	C-N-CA	-13.48	103.65	120.23
1	A	1378	GLU	CA-C-N	-7.33	114.97	122.74
1	A	1378	GLU	C-N-CA	-7.33	114.97	122.74
1	A	1597	GLU	CA-C-N	-7.30	111.25	119.28
1	A	1597	GLU	C-N-CA	-7.30	111.25	119.28
1	A	1640	VAL	N-CA-C	-6.87	103.78	110.72
1	A	1384	ILE	N-CA-C	-6.15	103.68	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1605	THR	N-CA-C	-5.87	104.97	111.36
1	A	1356	THR	OG1-CB-CG2	-5.85	97.59	109.30
1	A	1399	ASN	N-CA-C	5.84	118.43	111.71
1	A	1497	ILE	N-CA-CB	5.29	117.74	110.54
1	A	1608	GLU	CA-CB-CG	-5.20	103.71	114.10
1	A	1492	LEU	N-CA-C	5.06	116.80	111.28
1	A	1453	ASN	N-CA-C	5.05	119.08	113.02

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	2270	0	2265	54	0
2	A	185	0	0	10	0
All	All	2455	0	2265	54	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 12.

All (54) 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: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:1361:LYS:NZ	2:A:2025:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:1613:LEU:C	1:A:1613:LEU:HD23	2.39	0.47
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:1513:SER:C	1:A:1515:ARG:H	2.26	0.42
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:HB2	1:A:1522:LYS:HE2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	306/309 (99%)	288 (94%)	11 (4%)	7 (2%)	5 2

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 [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	243/243 (100%)	225 (93%)	18 (7%)	13 9

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1352	ILE
1	A	1368	ARG
1	A	1461	LEU
1	A	1462	VAL
1	A	1465	THR
1	A	1472	GLN
1	A	1479	GLN
1	A	1493	SER
1	A	1497	ILE
1	A	1505	LEU
1	A	1515	ARG
1	A	1522	LYS
1	A	1536	THR
1	A	1553	GLU
1	A	1572	LEU
1	A	1575	PHE
1	A	1647	LEU
1	A	1658	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1358	HIS
1	A	1360	GLN
1	A	1412	GLN
1	A	1418	ASN
1	A	1442	GLN
1	A	1466	GLN
1	A	1527	GLN
1	A	1557	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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 ⓘ

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, 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	308/309 (99%)	0.71	60 (19%) 3 3	15, 34, 68, 80	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1579	PRO	5.2
1	A	1521	ALA	5.1
1	A	1517	ALA	5.0
1	A	1485	GLY	4.5
1	A	1467	PHE	4.4
1	A	1519	PRO	4.3
1	A	1520	THR	4.2
1	A	1581	PHE	4.2
1	A	1464	PRO	4.1
1	A	1462	VAL	3.5
1	A	1468	ALA	3.5
1	A	1498	VAL	3.4
1	A	1352	ILE	3.4
1	A	1573	SER	3.3
1	A	1465	THR	3.3
1	A	1497	ILE	3.3
1	A	1495	ALA	3.3
1	A	1499	ALA	3.3
1	A	1492	LEU	3.2
1	A	1514	ALA	3.2
1	A	1500	LYS	3.2
1	A	1574	ALA	3.1
1	A	1484	PRO	3.1
1	A	1547	ASP	3.0
1	A	1473	ALA	2.9
1	A	1524	GLN	2.9
1	A	1496	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1476	MET	2.9
1	A	1503	SER	2.9
1	A	1470	ALA	2.9
1	A	1507	ASN	2.8
1	A	1577	SER	2.8
1	A	1513	SER	2.8
1	A	1491	VAL	2.8
1	A	1516	THR	2.7
1	A	1471	ASN	2.7
1	A	1551	THR	2.6
1	A	1575	PHE	2.6
1	A	1548	GLY	2.6
1	A	1537	ALA	2.6
1	A	1576	ALA	2.6
1	A	1502	THR	2.5
1	A	1561	ALA	2.5
1	A	1463	GLU	2.5
1	A	1386	ASP	2.4
1	A	1479	GLN	2.4
1	A	1412	GLN	2.4
1	A	1487	THR	2.4
1	A	1572	LEU	2.4
1	A	1578	ASN	2.4
1	A	1583	SER	2.4
1	A	1481	LEU	2.3
1	A	1523	ARG	2.3
1	A	1461	LEU	2.2
1	A	1566	LEU	2.2
1	A	1486	CYS	2.2
1	A	1482	GLY	2.1
1	A	1512	ALA	2.1
1	A	1474	ILE	2.1
1	A	1505	LEU	2.1

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 oligosaccharides 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.