Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2023 – 04:07 pm GMT

PDB ID	:	2X0C
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 (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:

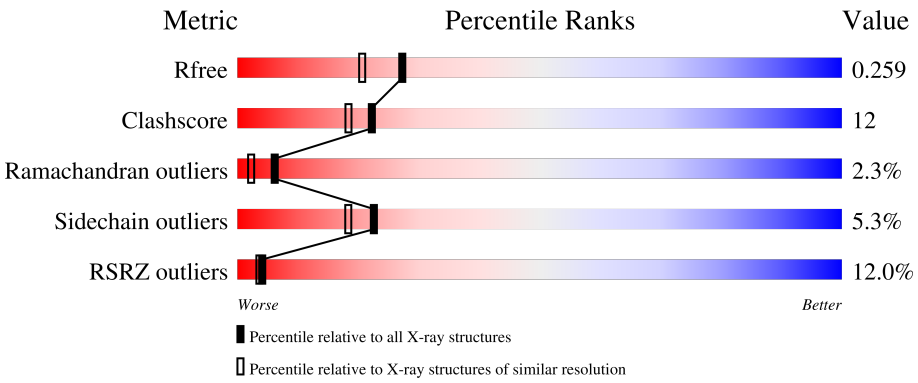
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	12% 77% 18% 5%

2 Entry composition (i)

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
			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.

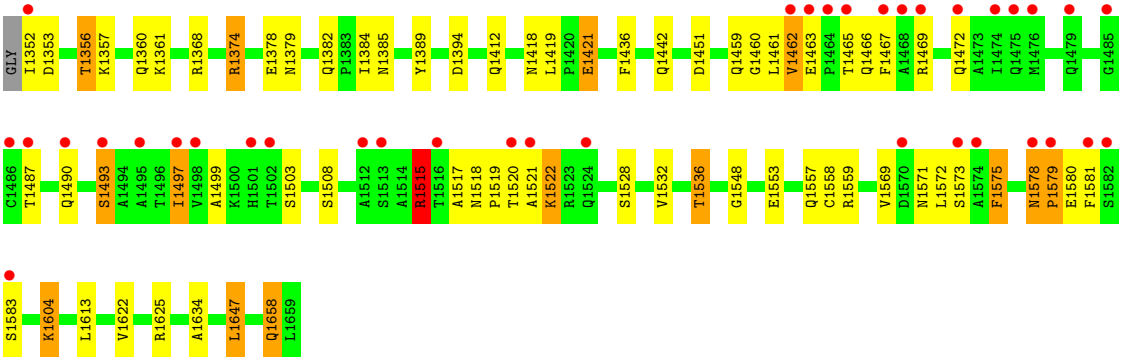
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	185	185	185	0	0

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: TALIN-1

Chain A:



4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [1]	2.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.212 , 0.264 0.210 , 0.259	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 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	
		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(^{o})	Ideal(^{o})
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 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	A	2270	0	2265	53	0
2	A	185	0	0	10	0
All	All	2455	0	2265	53	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 (53) 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: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	Interatomic distance (Å)	Clash overlap (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:HB2	1:A:1522:LYS:HE2	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 (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%)	6 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%)	230 (95%)	13 (5%)	22 18

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

Sometimes 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
1	A	1442	GLN
1	A	1466	GLN
1	A	1527	GLN
1	A	1557	GLN

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, 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%)	0.62	37 (12%) 4 3	15, 34, 68, 80	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1465	THR	5.6
1	A	1468	ALA	5.2
1	A	1467	PHE	4.9
1	A	1497	ILE	4.9
1	A	1521	ALA	4.7
1	A	1485	GLY	4.4
1	A	1520	THR	4.3
1	A	1498	VAL	4.2
1	A	1476	MET	4.1
1	A	1502	THR	3.7
1	A	1581	PHE	3.7
1	A	1513	SER	3.5
1	A	1472	GLN	3.5
1	A	1479	GLN	3.3
1	A	1464	PRO	3.3
1	A	1579	PRO	3.1
1	A	1474	ILE	2.9
1	A	1495	ALA	2.8
1	A	1493	SER	2.8
1	A	1516	THR	2.7
1	A	1574	ALA	2.7
1	A	1573	SER	2.6
1	A	1578	ASN	2.6
1	A	1512	ALA	2.5
1	A	1475	GLN	2.4
1	A	1487	THR	2.4
1	A	1462	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1352	ILE	2.4
1	A	1524	GLN	2.4
1	A	1486	CYS	2.3
1	A	1582	SER	2.3
1	A	1463	GLU	2.2
1	A	1583	SER	2.2
1	A	1469	ARG	2.2
1	A	1490	GLN	2.2
1	A	1570	ASP	2.1
1	A	1501	HIS	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 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.