Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KGX
Title	:	HADDOCK structure of the talin F3 domain in complex with talin 1655-1822
Authors	:	Goult, B.T.; Gingras, A.R.; Bate, N.; Critchley, D.R.; Barsukov, I.L.
Deposited on	:	2009-03-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

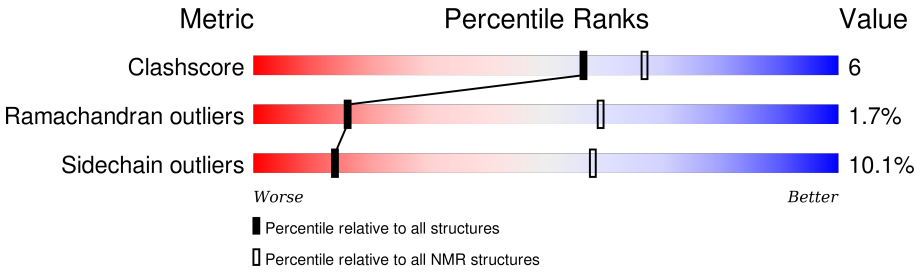
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	174	59% 38% .
2	B	91	73% 26% .

2 Ensemble composition and analysis

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2459 atoms, of which 445 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Talin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			1549	785	274	218	265	7	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1649	GLY	-	EXPRESSION TAG	UNP P26039
A	1650	ILE	-	EXPRESSION TAG	UNP P26039
A	1651	ASP	-	EXPRESSION TAG	UNP P26039
A	1652	PRO	-	EXPRESSION TAG	UNP P26039
A	1653	PHE	-	EXPRESSION TAG	UNP P26039
A	1654	THR	-	EXPRESSION TAG	UNP P26039

- Molecule 2 is a protein called MKIAA1027 protein.

Mol	Chain	Residues	Atoms						Trace
2	B	91	Total	C	H	N	O	S	0
			910	478	171	120	139	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	336	SER	CYS	ENGINEERED	UNP Q80TM2

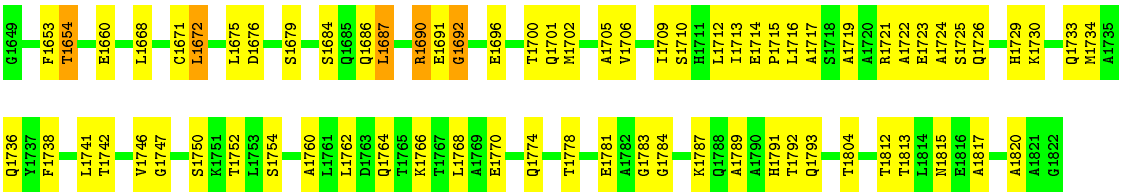
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

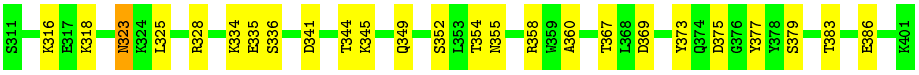
- Molecule 1: Talin-1

Chain A:



- Molecule 2: MKIAA1027 protein

Chain B:



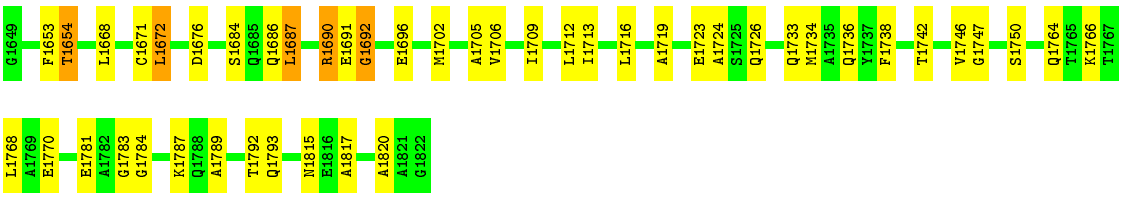
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

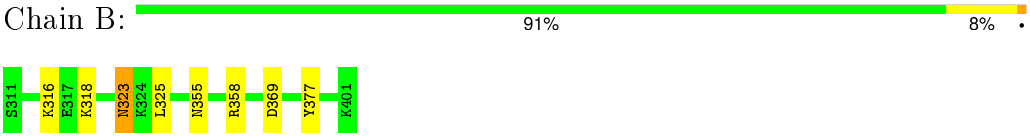
- Molecule 1: Talin-1

Chain A:



• Molecule 2: MKIAA1027 protein

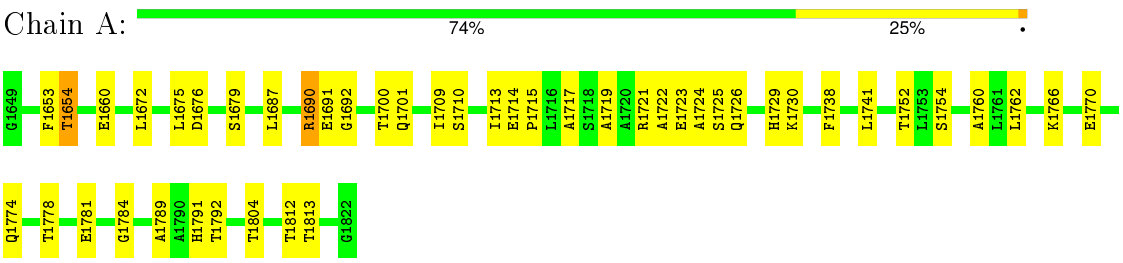
Chain B:



4.2.2 Score per residue for model 2

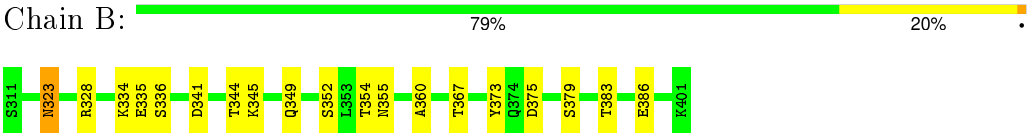
• Molecule 1: Talin-1

Chain A:



• Molecule 2: MKIAA1027 protein

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Protein-protein docking.*

Of the 200 calculated structures, 2 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	refinement	2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1275	274	1262	24±6
2	B	739	171	759	4±0
All	All	4028	890	4042	51

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 6.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1690:ARG:HA	1:A:1747:GLY:HA2	0.84	1.48	1	1
1:A:1712:LEU:HD11	1:A:1734:MET:HB2	0.65	1.68	1	1
1:A:1789:ALA:HB1	1:A:1792:THR:HB	0.65	1.69	1	2
1:A:1716:LEU:HD13	1:A:1734:MET:HE3	0.63	1.69	1	1
1:A:1719:ALA:HA	1:A:1723:GLU:HB2	0.63	1.71	2	2
1:A:1709:ILE:O	1:A:1713:ILE:HG13	0.60	1.96	1	2
1:A:1653:PHE:CZ	1:A:1781:GLU:HA	0.58	2.33	1	1
1:A:1770:GLU:HB3	2:B:323:ASN:HB3	0.57	1.76	2	2
2:B:328:ARG:HD2	2:B:341:ASP:HA	0.57	1.75	2	1
1:A:1714:GLU:HB2	1:A:1715:PRO:HD3	0.55	1.79	2	1
1:A:1723:GLU:HB3	1:A:1726:GLN:HB2	0.55	1.79	1	2
1:A:1676:ASP:HA	1:A:1766:LYS:HE2	0.54	1.80	1	2
1:A:1653:PHE:O	1:A:1654:THR:HB	0.54	2.02	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1742:THR:O	1:A:1746:VAL:HG23	0.53	2.04	1	1
1:A:1724:ALA:HB2	1:A:1784:GLY:HA2	0.52	1.79	2	1
1:A:1781:GLU:HB2	1:A:1792:THR:HG21	0.52	1.81	2	2
1:A:1726:GLN:O	1:A:1730:LYS:HG2	0.49	2.07	2	1
1:A:1687:LEU:HD12	1:A:1750:SER:HB2	0.49	1.84	1	1
2:B:316:LYS:HD3	2:B:325:LEU:HB3	0.49	1.83	1	1
1:A:1690:ARG:HA	1:A:1747:GLY:CA	0.48	2.31	1	1
1:A:1690:ARG:CA	1:A:1747:GLY:HA2	0.48	2.32	1	1
1:A:1733:GLN:O	1:A:1736:GLN:HG2	0.48	2.09	1	1
1:A:1679:SER:HA	1:A:1762:LEU:HD21	0.47	1.86	2	1
1:A:1684:SER:HB3	1:A:1686:GLN:HE21	0.47	1.70	1	1
1:A:1705:ALA:O	1:A:1709:ILE:HG13	0.47	2.10	1	1
1:A:1702:MET:O	1:A:1706:VAL:HG23	0.47	2.10	1	1
1:A:1789:ALA:O	1:A:1793:GLN:HG2	0.46	2.11	1	1
1:A:1724:ALA:HB2	1:A:1784:GLY:HA3	0.45	1.87	1	1
1:A:1690:ARG:NH1	1:A:1692:GLY:HA2	0.45	2.27	1	1
1:A:1717:ALA:O	1:A:1721:ARG:HG2	0.44	2.12	2	1
1:A:1726:GLN:HA	1:A:1729:HIS:ND1	0.44	2.28	2	1
2:B:358:ARG:HG3	2:B:369:ASP:HB3	0.43	1.89	1	1
1:A:1672:LEU:HA	1:A:1672:LEU:HD13	0.43	1.72	1	1
1:A:1668:LEU:HD12	1:A:1671:CYS:SG	0.43	2.54	1	1
1:A:1766:LYS:O	1:A:1770:GLU:HG3	0.42	2.14	2	1
1:A:1712:LEU:HD21	1:A:1734:MET:HA	0.42	1.90	1	1
1:A:1760:ALA:HB2	2:B:360:ALA:HB1	0.42	1.91	2	1
2:B:341:ASP:O	2:B:345:LYS:HA	0.42	2.14	2	1
1:A:1817:ALA:HA	1:A:1820:ALA:HB3	0.41	1.91	1	1
1:A:1709:ILE:HD13	1:A:1738:PHE:CE1	0.41	2.49	1	1
1:A:1710:SER:HA	1:A:1713:ILE:HD12	0.41	1.91	2	1
1:A:1716:LEU:HD13	1:A:1734:MET:CE	0.40	2.44	1	1
1:A:1764:GLN:O	1:A:1768:LEU:HB2	0.40	2.16	1	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	172/174 (99%)	160±1 (93±0%)	9±1 (5±0%)	4±0 (2±0%)	12 51
2	B	89/91 (98%)	82±2 (92±2%)	7±1 (8±1%)	1±1 (1±1%)	34 78
All	All	522/530 (98%)	482 (92%)	31 (6%)	9 (2%)	16 59

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	1654	THR	2
1	A	1692	GLY	2
1	A	1690	ARG	2
1	A	1783	GLY	1
2	B	373	TYR	1
1	A	1722	ALA	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	132/132 (100%)	120±7 (91±5%)	13±7 (9±5%)	15 60
2	B	81/81 (100%)	72±5 (89±6%)	9±5 (11±6%)	12 55
All	All	426/426 (100%)	383 (90%)	43 (10%)	14 58

All 38 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	1672	LEU	2
1	A	1687	LEU	2
2	B	355	ASN	2
2	B	323	ASN	2
1	A	1691	GLU	2
1	A	1660	GLU	1
1	A	1754	SER	1
1	A	1696	GLU	1
1	A	1741	LEU	1
2	B	349	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	1778	THR	1
2	B	386	GLU	1
1	A	1813	THR	1
2	B	367	THR	1
1	A	1700	THR	1
2	B	379	SER	1
2	B	334	LYS	1
2	B	383	THR	1
1	A	1804	THR	1
1	A	1774	GLN	1
2	B	354	THR	1
2	B	344	THR	1
1	A	1690	ARG	1
1	A	1752	THR	1
2	B	318	LYS	1
2	B	335	GLU	1
1	A	1675	LEU	1
2	B	377	TYR	1
2	B	336	SER	1
1	A	1738	PHE	1
1	A	1725	SER	1
2	B	352	SER	1
1	A	1791	HIS	1
2	B	375	ASP	1
1	A	1787	LYS	1
1	A	1815	ASN	1
1	A	1812	THR	1
1	A	1701	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided