



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 08:19 AM UTC

PDB ID : 2KBB / pdb_00002kbb
Title : Solution Structure of the R9 Domain of Talin
Authors : Goult, B.T.; Gingras, A.R.; Bate, N.; Critchley, D.R.; Barsukov, I.L.
Deposited on : 2008-11-24

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

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

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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

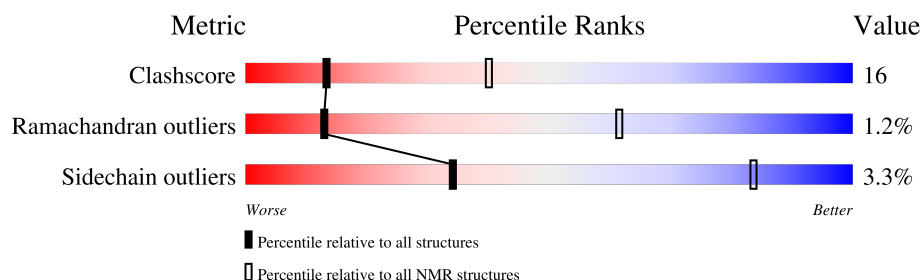
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	174	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1656-A:1753, A:1757-A:1822 (164)	0.60	7

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 6, 7, 9, 11, 12, 15, 17, 18, 19
2	3, 5, 8, 13
3	14, 16, 20
Single-model clusters	10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2540 atoms, of which 1265 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
			2540	785	1265	218	265	7	

There are 6 discrepancies between the modelled and reference sequences:

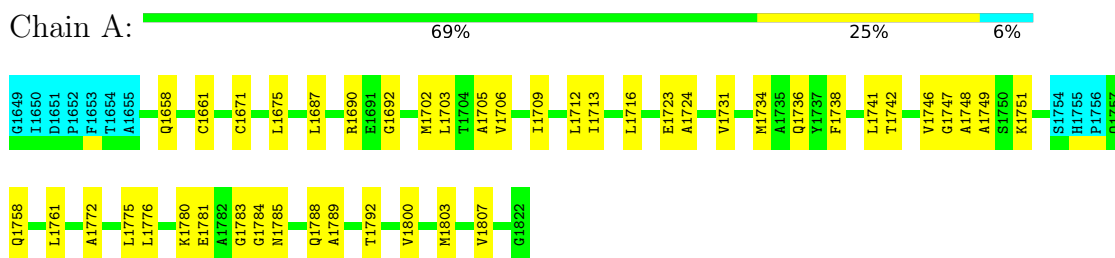
Chain	Residue	Modelled	Actual	Comment	Reference
A	1649	GLY	-	expression tag	UNP P26039
A	1650	ILE	-	expression tag	UNP P26039
A	1651	ASP	-	expression tag	UNP P26039
A	1652	PRO	-	expression tag	UNP P26039
A	1653	PHE	-	expression tag	UNP P26039
A	1654	THR	-	expression tag	UNP P26039

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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

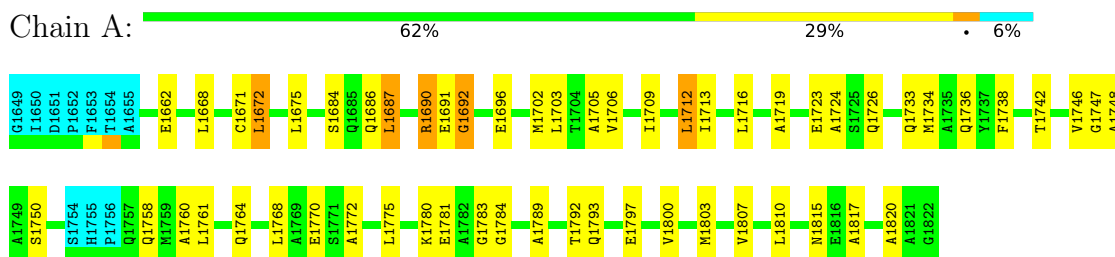


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

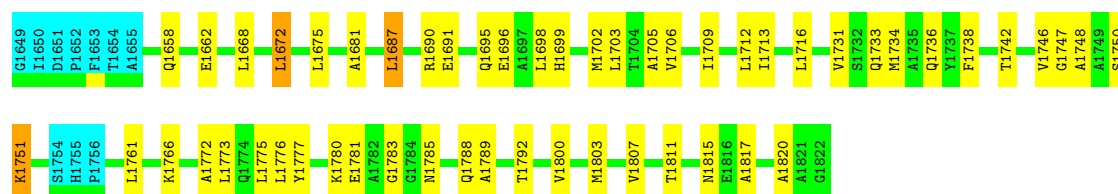
- Molecule 1: Talin-1



4.2.2 Score per residue for model 2

- Molecule 1: Talin-1

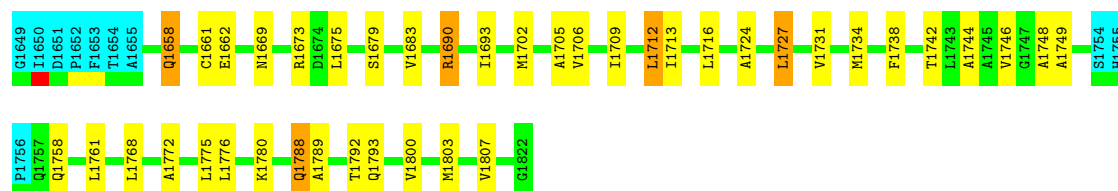




4.2.3 Score per residue for model 3

- Molecule 1: Talin-1

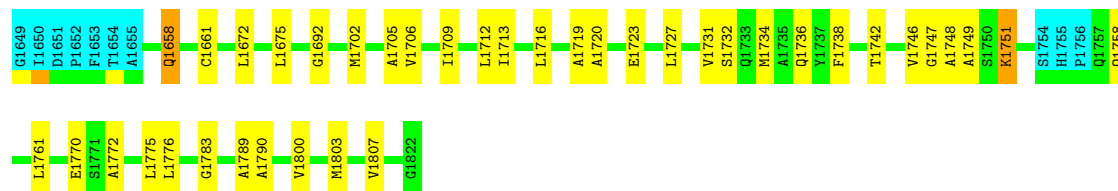
Chain A: 71% 21% 6%



4.2.4 Score per residue for model 4

- Molecule 1: Talin-1

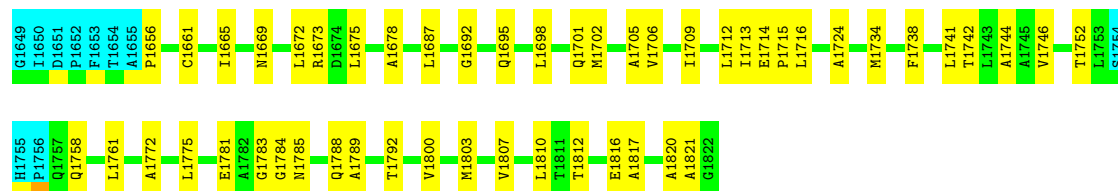
Chain A: 72% 21% 6%



4.2.5 Score per residue for model 5

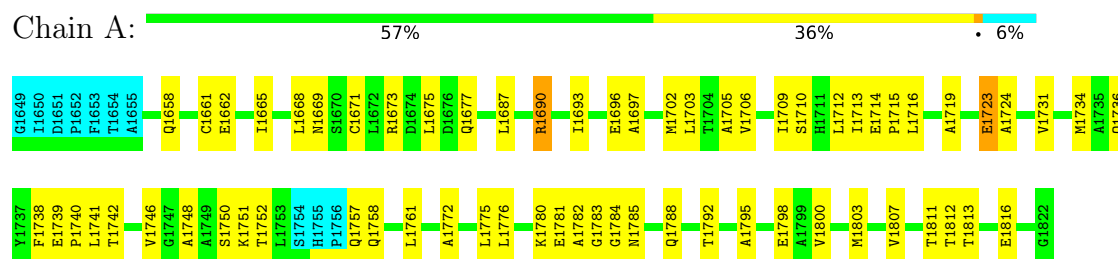
- Molecule 1: Talin-1

Chain A: 66% 29% 6%



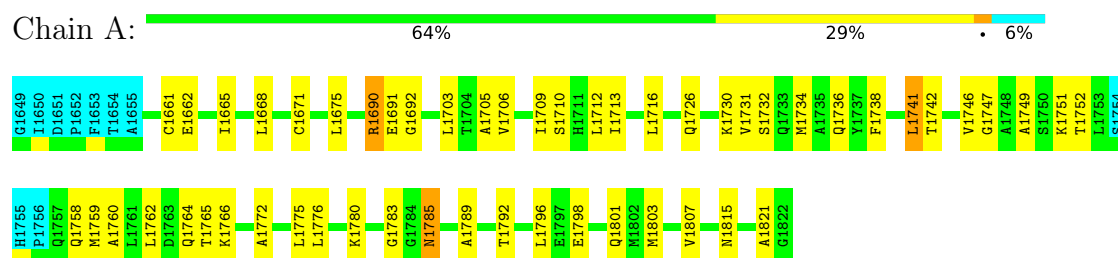
4.2.6 Score per residue for model 6

- Molecule 1: Talin-1



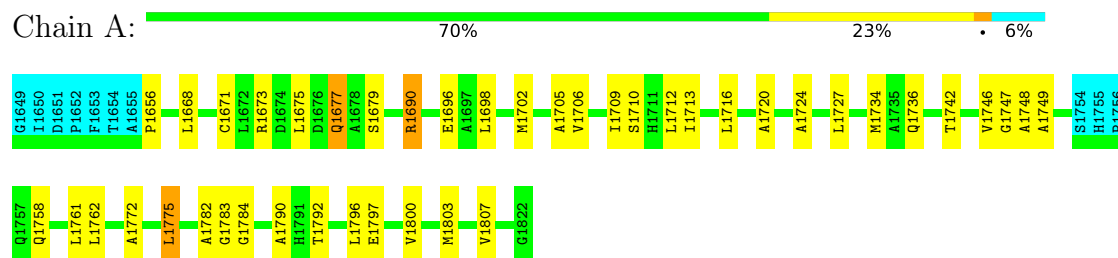
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Talin-1



4.2.8 Score per residue for model 8

- Molecule 1: Talin-1





4.2.10 Score per residue for model 10

- Molecule 1: Talin-1

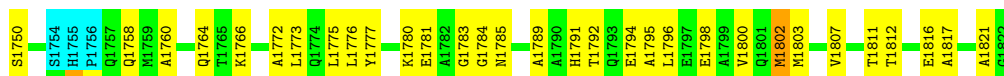
Chain A: 66% 26% 6%



4.2.11 Score per residue for model 11

- Molecule 1: Talin-1

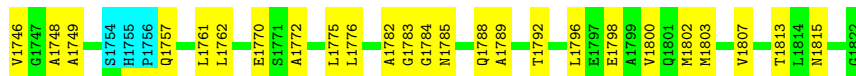
Chain A: 59% 34% 6%



4.2.12 Score per residue for model 12

- Molecule 1: Talin-1

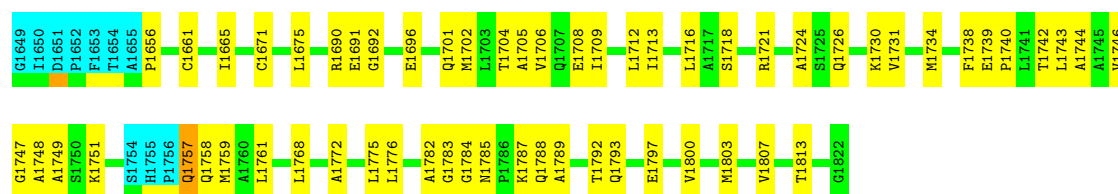
Chain A: 61% 33% 6%



4.2.13 Score per residue for model 13

- Molecule 1: Talin-1

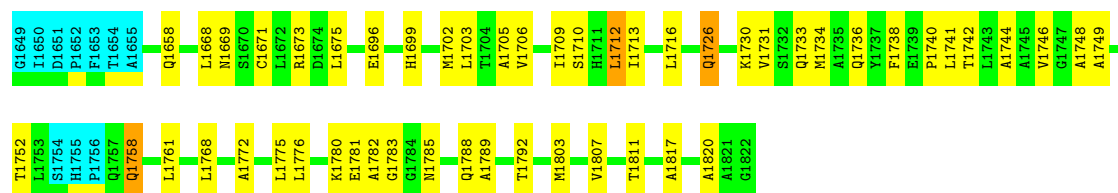
Chain A: 60% 33% 6%



4.2.14 Score per residue for model 14

- Molecule 1: Talin-1

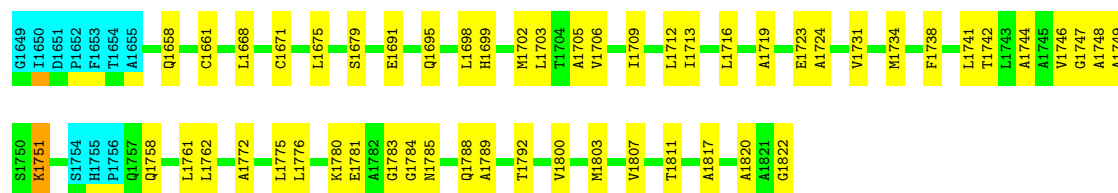
Chain A: 65% 28% 6%



4.2.15 Score per residue for model 15

- Molecule 1: Talin-1

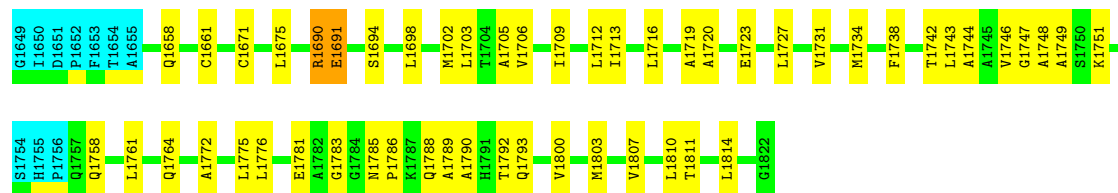
Chain A: 64% 30% 6%



4.2.16 Score per residue for model 16

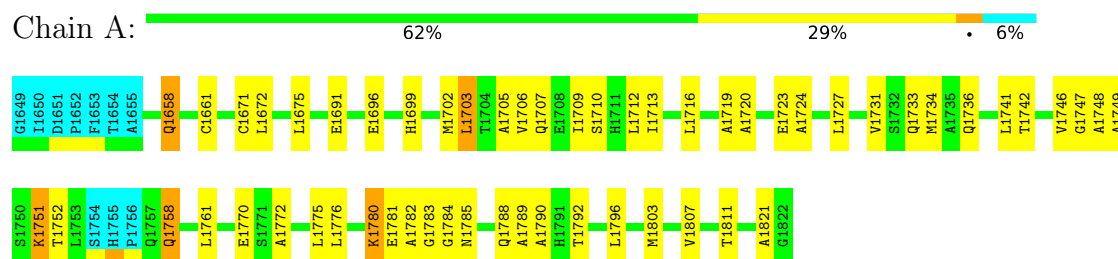
- Molecule 1: Talin-1

Chain A: 64% 29% 6%



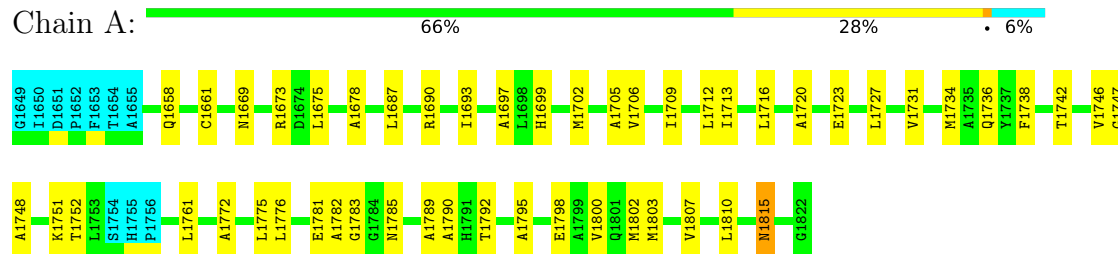
4.2.17 Score per residue for model 17

- Molecule 1: Talin-1



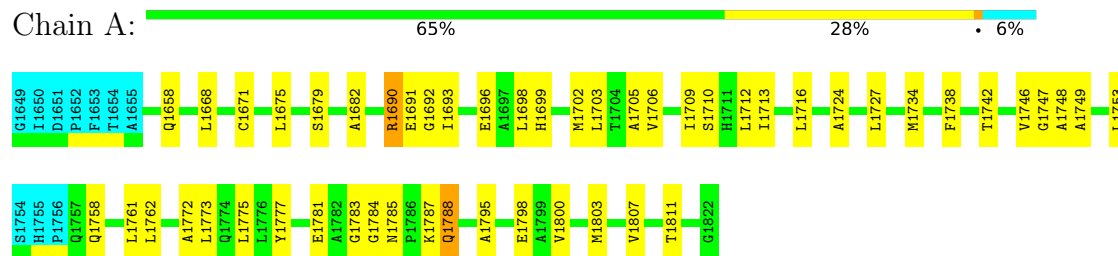
4.2.18 Score per residue for model 18

- Molecule 1: Talin-1



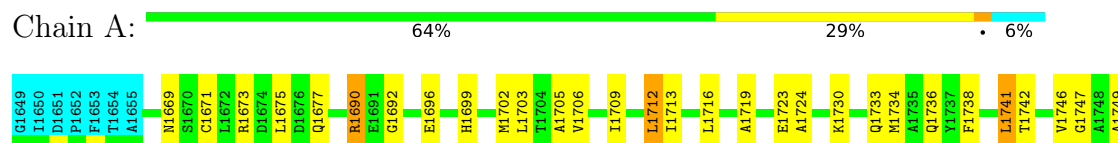
4.2.19 Score per residue for model 19

- Molecule 1: Talin-1



4.2.20 Score per residue for model 20

- Molecule 1: Talin-1



T1752	L1753	S1754	H1755	P1756	Q1757	Q1758	L1762	T1765	A1772	L1775	K1780	E1781	A1782	G1783	G1784	Q1788	A1789	T1792	A1795	E1798	A1799	V1800	M1803	V1807	T1811	T1812	N1815	E1816	A1821	G1822
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING, MOLECULAR DYNAMICS, TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 20 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
ARIA	refinement	1.2
CYANA	structure solution	2.1

No chemical shift data was provided.

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	1202	1198	1198	39±5
All	All	24040	23960	23960	779

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1785:ASN:HD21	1:A:1788:GLN:HB2	0.87	1.30	5	6
1:A:1690:ARG:HA	1:A:1747:GLY:HA2	0.85	1.48	1	3
1:A:1687:LEU:HD12	1:A:1750:SER:HB2	0.77	1.57	2	2
1:A:1817:ALA:HA	1:A:1820:ALA:HB3	0.77	1.55	2	6
1:A:1789:ALA:HA	1:A:1792:THR:HB	0.74	1.58	3	2
1:A:1757:GLN:HE21	1:A:1757:GLN:HA	0.74	1.40	13	1
1:A:1789:ALA:HB1	1:A:1792:THR:HB	0.73	1.59	16	13
1:A:1668:LEU:HD12	1:A:1671:CYS:SG	0.72	2.24	8	7
1:A:1749:ALA:HA	1:A:1758:GLN:HB2	0.72	1.61	14	2
1:A:1782:ALA:HA	1:A:1789:ALA:HB2	0.71	1.61	17	2
1:A:1712:LEU:HD11	1:A:1734:MET:HB2	0.70	1.62	5	20
1:A:1690:ARG:HD3	1:A:1692:GLY:H	0.69	1.47	20	1
1:A:1726:GLN:HE21	1:A:1726:GLN:HA	0.69	1.48	14	1
1:A:1713:ILE:HG22	1:A:1800:VAL:HG23	0.69	1.63	9	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1706:VAL:HG12	1:A:1807:VAL:HG13	0.68	1.65	6	17
1:A:1731:VAL:HG13	1:A:1776:LEU:HD22	0.68	1.66	6	15
1:A:1713:ILE:HD13	1:A:1803:MET:HB3	0.67	1.67	17	19
1:A:1698:LEU:HD22	1:A:1744:ALA:HA	0.66	1.67	16	1
1:A:1795:ALA:HA	1:A:1798:GLU:HG2	0.65	1.68	9	4
1:A:1709:ILE:O	1:A:1713:ILE:HG13	0.65	1.92	19	20
1:A:1774:GLN:HE21	1:A:1774:GLN:HA	0.64	1.51	9	1
1:A:1716:LEU:HD22	1:A:1775:LEU:HD11	0.64	1.69	1	20
1:A:1675:LEU:HG	1:A:1742:THR:HG23	0.63	1.70	6	20
1:A:1690:ARG:HG3	1:A:1692:GLY:H	0.63	1.53	11	1
1:A:1749:ALA:HA	1:A:1758:GLN:CG	0.63	2.24	10	8
1:A:1785:ASN:ND2	1:A:1788:GLN:HB2	0.62	2.09	10	5
1:A:1677:GLN:HA	1:A:1677:GLN:HE21	0.62	1.54	8	1
1:A:1781:GLU:HB2	1:A:1792:THR:HG21	0.62	1.72	2	10
1:A:1742:THR:O	1:A:1746:VAL:HG23	0.62	1.93	12	20
1:A:1785:ASN:HD21	1:A:1788:GLN:HB3	0.62	1.53	15	2
1:A:1690:ARG:HH11	1:A:1691:GLU:HB2	0.61	1.54	13	1
1:A:1749:ALA:HA	1:A:1758:GLN:HG3	0.61	1.72	10	5
1:A:1662:GLU:HB2	1:A:1780:LYS:HD2	0.61	1.72	1	4
1:A:1749:ALA:HB2	1:A:1762:LEU:HD22	0.61	1.72	20	5
1:A:1696:GLU:HA	1:A:1699:HIS:CD2	0.60	2.31	20	1
1:A:1733:GLN:O	1:A:1736:GLN:HG2	0.59	1.97	10	7
1:A:1699:HIS:CE1	1:A:1815:ASN:HA	0.58	2.33	18	3
1:A:1747:GLY:O	1:A:1751:LYS:HG3	0.58	1.98	16	2
1:A:1661:CYS:HA	1:A:1731:VAL:HG11	0.57	1.73	16	13
1:A:1747:GLY:O	1:A:1751:LYS:HG2	0.57	1.99	15	4
1:A:1719:ALA:HA	1:A:1723:GLU:HB2	0.57	1.76	1	7
1:A:1713:ILE:HG12	1:A:1734:MET:HE2	0.57	1.75	10	13
1:A:1687:LEU:HD11	1:A:1746:VAL:HG12	0.57	1.76	2	1
1:A:1710:SER:HA	1:A:1713:ILE:HD12	0.57	1.76	8	6
1:A:1690:ARG:HD3	1:A:1693:ILE:H	0.57	1.59	3	1
1:A:1710:SER:HB2	1:A:1807:VAL:HG11	0.56	1.77	12	8
1:A:1675:LEU:HB3	1:A:1766:LYS:HB2	0.56	1.77	11	2
1:A:1713:ILE:HD13	1:A:1803:MET:CB	0.56	2.30	10	19
1:A:1772:ALA:HB2	1:A:1803:MET:HE3	0.56	1.77	8	20
1:A:1690:ARG:HD3	1:A:1698:LEU:HD21	0.56	1.78	11	3
1:A:1701:GLN:HE21	1:A:1744:ALA:HB2	0.56	1.61	5	1
1:A:1689:PRO:HA	1:A:1750:SER:HB3	0.55	1.79	11	1
1:A:1732:SER:O	1:A:1736:GLN:HG3	0.55	2.01	4	2
1:A:1705:ALA:HB3	1:A:1741:LEU:HD21	0.55	1.79	15	3
1:A:1703:LEU:HD22	1:A:1815:ASN:HD21	0.54	1.60	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1690:ARG:HB3	1:A:1751:LYS:HB2	0.54	1.79	18	1
1:A:1803:MET:O	1:A:1807:VAL:HG23	0.54	2.03	18	19
1:A:1748:ALA:HB3	1:A:1761:LEU:HD11	0.54	1.78	16	14
1:A:1703:LEU:HD23	1:A:1811:THR:HG23	0.54	1.79	17	9
1:A:1706:VAL:HG22	1:A:1807:VAL:HG13	0.53	1.79	10	1
1:A:1724:ALA:HB2	1:A:1784:GLY:HA3	0.53	1.80	17	11
1:A:1782:ALA:HB2	1:A:1792:THR:HG22	0.53	1.80	13	5
1:A:1675:LEU:HD13	1:A:1766:LYS:HA	0.53	1.80	9	2
1:A:1723:GLU:HB3	1:A:1726:GLN:HB2	0.53	1.80	1	1
1:A:1789:ALA:HB1	1:A:1793:GLN:HG3	0.53	1.79	3	2
1:A:1812:THR:O	1:A:1816:GLU:HG3	0.53	2.04	11	5
1:A:1705:ALA:O	1:A:1709:ILE:HG13	0.52	2.04	2	20
1:A:1709:ILE:HD13	1:A:1738:PHE:CE1	0.52	2.40	10	12
1:A:1741:LEU:HD22	1:A:1765:THR:HG23	0.52	1.81	7	3
1:A:1789:ALA:HB1	1:A:1792:THR:CB	0.52	2.30	16	1
1:A:1698:LEU:CD2	1:A:1744:ALA:HA	0.52	2.35	16	1
1:A:1720:ALA:HA	1:A:1727:LEU:HD22	0.52	1.80	8	4
1:A:1733:GLN:O	1:A:1736:GLN:HG3	0.52	2.05	14	1
1:A:1703:LEU:HG	1:A:1815:ASN:HD21	0.52	1.64	1	2
1:A:1681:ALA:HB3	1:A:1687:LEU:HD23	0.52	1.81	11	4
1:A:1716:LEU:HD13	1:A:1734:MET:HE3	0.51	1.81	10	19
1:A:1690:ARG:HA	1:A:1747:GLY:CA	0.51	2.31	1	2
1:A:1726:GLN:O	1:A:1730:LYS:HG2	0.51	2.05	13	3
1:A:1691:GLU:H	1:A:1691:GLU:CD	0.51	2.12	19	1
1:A:1782:ALA:HB2	1:A:1792:THR:CG2	0.51	2.36	13	1
1:A:1757:GLN:OE1	1:A:1813:THR:HG23	0.51	2.06	12	2
1:A:1696:GLU:HA	1:A:1699:HIS:ND1	0.51	2.20	19	3
1:A:1704:THR:HA	1:A:1707:GLN:HE21	0.51	1.65	12	1
1:A:1679:SER:HA	1:A:1762:LEU:HD21	0.51	1.83	8	4
1:A:1671:CYS:HB3	1:A:1742:THR:OG1	0.51	2.06	9	8
1:A:1748:ALA:O	1:A:1752:THR:HB	0.50	2.06	17	3
1:A:1682:ALA:HB2	1:A:1749:ALA:HB1	0.50	1.82	19	1
1:A:1669:ASN:O	1:A:1673:ARG:HG2	0.50	2.06	3	3
1:A:1773:LEU:HG	1:A:1777:TYR:CE2	0.50	2.42	19	3
1:A:1698:LEU:HD22	1:A:1744:ALA:CA	0.50	2.35	16	1
1:A:1709:ILE:HD13	1:A:1738:PHE:CE2	0.50	2.42	9	6
1:A:1702:MET:HA	1:A:1741:LEU:CD2	0.50	2.37	12	2
1:A:1658:GLN:OE1	1:A:1658:GLN:HA	0.50	2.07	4	1
1:A:1726:GLN:HB3	1:A:1730:LYS:HE2	0.50	1.84	7	1
1:A:1760:ALA:O	1:A:1764:GLN:HG2	0.50	2.07	7	1
1:A:1702:MET:O	1:A:1706:VAL:HG23	0.49	2.07	9	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1713:ILE:HD11	1:A:1803:MET:HE2	0.49	1.84	7	3
1:A:1694:SER:O	1:A:1698:LEU:HG	0.49	2.08	16	1
1:A:1703:LEU:HD13	1:A:1811:THR:HG23	0.49	1.83	20	1
1:A:1789:ALA:HA	1:A:1792:THR:CB	0.49	2.34	3	1
1:A:1662:GLU:HA	1:A:1665:ILE:HB	0.49	1.85	6	1
1:A:1690:ARG:HB3	1:A:1747:GLY:CA	0.48	2.37	8	2
1:A:1656:PRO:O	1:A:1724:ALA:HB1	0.48	2.08	12	5
1:A:1786:PRO:HB3	1:A:1793:GLN:NE2	0.48	2.24	16	1
1:A:1709:ILE:O	1:A:1712:LEU:HG	0.48	2.07	8	7
1:A:1720:ALA:HA	1:A:1727:LEU:HD13	0.48	1.86	17	2
1:A:1706:VAL:CG1	1:A:1807:VAL:HG13	0.48	2.38	11	5
1:A:1658:GLN:HG3	1:A:1780:LYS:O	0.48	2.08	14	3
1:A:1690:ARG:NH1	1:A:1691:GLU:HB2	0.48	2.22	13	1
1:A:1794:GLU:HG3	1:A:1795:ALA:N	0.47	2.24	11	1
1:A:1672:LEU:HD11	1:A:1770:GLU:CG	0.47	2.38	4	2
1:A:1760:ALA:O	1:A:1764:GLN:HG3	0.47	2.09	11	2
1:A:1714:GLU:HB2	1:A:1715:PRO:CD	0.47	2.39	5	1
1:A:1691:GLU:HG3	1:A:1743:LEU:HD13	0.47	1.87	13	1
1:A:1690:ARG:CA	1:A:1747:GLY:HA2	0.47	2.32	1	1
1:A:1661:CYS:SG	1:A:1731:VAL:HG21	0.47	2.49	18	5
1:A:1717:ALA:O	1:A:1721:ARG:HG2	0.47	2.08	10	1
1:A:1701:GLN:OE1	1:A:1744:ALA:HB2	0.47	2.10	13	1
1:A:1713:ILE:CD1	1:A:1803:MET:HB3	0.47	2.38	14	8
1:A:1661:CYS:O	1:A:1665:ILE:HG13	0.47	2.10	7	3
1:A:1736:GLN:O	1:A:1740:PRO:HD2	0.47	2.10	14	2
1:A:1780:LYS:HE2	1:A:1781:GLU:OE1	0.47	2.09	9	1
1:A:1696:GLU:H	1:A:1696:GLU:CD	0.47	2.17	10	1
1:A:1733:GLN:HA	1:A:1736:GLN:NE2	0.47	2.25	12	1
1:A:1791:HIS:O	1:A:1794:GLU:HG2	0.47	2.10	11	1
1:A:1703:LEU:O	1:A:1707:GLN:HG3	0.47	2.10	12	2
1:A:1798:GLU:O	1:A:1802:MET:HG2	0.46	2.10	12	1
1:A:1669:ASN:O	1:A:1673:ARG:HG3	0.46	2.10	20	3
1:A:1789:ALA:O	1:A:1793:GLN:HG2	0.46	2.11	1	1
1:A:1748:ALA:HA	1:A:1751:LYS:HB3	0.46	1.87	9	1
1:A:1749:ALA:O	1:A:1758:GLN:HG3	0.46	2.09	10	1
1:A:1690:ARG:HH11	1:A:1743:LEU:HA	0.46	1.71	16	1
1:A:1810:LEU:O	1:A:1814:LEU:HG	0.46	2.10	16	1
1:A:1758:GLN:HG2	1:A:1759:MET:N	0.46	2.24	7	1
1:A:1690:ARG:HD3	1:A:1691:GLU:N	0.46	2.26	13	1
1:A:1668:LEU:HA	1:A:1671:CYS:SG	0.46	2.51	8	2
1:A:1690:ARG:NH2	1:A:1751:LYS:HA	0.46	2.26	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1757:GLN:NE2	1:A:1813:THR:HG23	0.46	2.26	13	1
1:A:1706:VAL:HG21	1:A:1810:LEU:HD23	0.46	1.86	18	2
1:A:1702:MET:SD	1:A:1744:ALA:HB3	0.46	2.50	14	6
1:A:1703:LEU:HA	1:A:1706:VAL:HG12	0.46	1.88	7	1
1:A:1693:ILE:HG12	1:A:1697:ALA:HB3	0.45	1.88	18	1
1:A:1671:CYS:HB2	1:A:1742:THR:OG1	0.45	2.11	8	5
1:A:1710:SER:HA	1:A:1713:ILE:CD1	0.45	2.41	10	2
1:A:1661:CYS:HB3	1:A:1780:LYS:HB2	0.45	1.86	6	1
1:A:1673:ARG:O	1:A:1677:GLN:HG2	0.45	2.12	8	2
1:A:1691:GLU:HG3	1:A:1743:LEU:HB3	0.45	1.88	9	1
1:A:1752:THR:HB	1:A:1758:GLN:HB3	0.45	1.89	14	3
1:A:1695:GLN:O	1:A:1698:LEU:HB2	0.45	2.12	2	3
1:A:1684:SER:HB3	1:A:1686:GLN:HE21	0.45	1.72	1	1
1:A:1738:PHE:CZ	1:A:1768:LEU:HG	0.44	2.47	13	4
1:A:1764:GLN:NE2	1:A:1810:LEU:HA	0.44	2.27	16	1
1:A:1690:ARG:HE	1:A:1693:ILE:HG22	0.44	1.72	19	1
1:A:1672:LEU:HD12	1:A:1766:LYS:HG3	0.44	1.88	2	1
1:A:1797:GLU:HA	1:A:1800:VAL:HG12	0.44	1.89	13	2
1:A:1752:THR:HG23	1:A:1821:ALA:CB	0.44	2.42	5	1
1:A:1672:LEU:HD11	1:A:1770:GLU:HG3	0.44	1.88	1	4
1:A:1690:ARG:NH1	1:A:1692:GLY:HA2	0.44	2.27	1	1
1:A:1712:LEU:HD21	1:A:1734:MET:HA	0.44	1.90	2	3
1:A:1749:ALA:CA	1:A:1758:GLN:HG3	0.44	2.42	10	1
1:A:1752:THR:HG23	1:A:1821:ALA:HB2	0.43	1.90	5	1
1:A:1690:ARG:HH21	1:A:1751:LYS:HA	0.43	1.73	6	1
1:A:1720:ALA:HB3	1:A:1796:LEU:HD21	0.43	1.90	12	2
1:A:1752:THR:O	1:A:1758:GLN:HG2	0.43	2.12	17	1
1:A:1687:LEU:HD21	1:A:1746:VAL:HG13	0.43	1.90	18	1
1:A:1757:GLN:OE1	1:A:1757:GLN:HA	0.43	2.13	6	1
1:A:1702:MET:SD	1:A:1741:LEU:HD12	0.43	2.54	5	1
1:A:1687:LEU:HD13	1:A:1688:ALA:O	0.43	2.13	11	1
1:A:1748:ALA:CB	1:A:1761:LEU:HD11	0.43	2.44	2	1
1:A:1678:ALA:HA	1:A:1687:LEU:HD13	0.43	1.90	5	2
1:A:1752:THR:O	1:A:1758:GLN:HB2	0.43	2.14	6	1
1:A:1798:GLU:HA	1:A:1801:GLN:HE21	0.43	1.74	7	1
1:A:1768:LEU:HD13	1:A:1806:ALA:HB3	0.43	1.91	9	1
1:A:1795:ALA:O	1:A:1798:GLU:HG2	0.43	2.14	20	1
1:A:1716:LEU:HD13	1:A:1734:MET:CE	0.42	2.44	1	8
1:A:1720:ALA:HB2	1:A:1727:LEU:HD13	0.42	1.90	9	1
1:A:1713:ILE:CG2	1:A:1800:VAL:HG23	0.42	2.40	8	1
1:A:1757:GLN:HE21	1:A:1757:GLN:CA	0.42	2.18	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1749:ALA:HB2	1:A:1762:LEU:HD13	0.42	1.92	19	1
1:A:1718:SER:O	1:A:1721:ARG:HG2	0.42	2.14	13	1
1:A:1724:ALA:O	1:A:1727:LEU:HB3	0.42	2.15	3	1
1:A:1695:GLN:HG2	1:A:1822:GLY:HA2	0.42	1.91	15	1
1:A:1812:THR:O	1:A:1816:GLU:HG2	0.42	2.15	10	1
1:A:1764:GLN:HE21	1:A:1810:LEU:HA	0.42	1.75	16	1
1:A:1703:LEU:O	1:A:1706:VAL:HG12	0.42	2.15	10	1
1:A:1690:ARG:HG2	1:A:1751:LYS:HD2	0.41	1.90	7	1
1:A:1787:LYS:HG2	1:A:1788:GLN:H	0.41	1.76	19	1
1:A:1739:GLU:HB3	1:A:1740:PRO:CD	0.41	2.45	13	2
1:A:1704:THR:HA	1:A:1707:GLN:OE1	0.41	2.16	9	1
1:A:1691:GLU:CD	1:A:1691:GLU:N	0.41	2.79	19	1
1:A:1687:LEU:HB3	1:A:1750:SER:HB3	0.41	1.91	6	1
1:A:1693:ILE:HD11	1:A:1697:ALA:HB1	0.41	1.92	6	1
1:A:1690:ARG:HD2	1:A:1751:LYS:HD2	0.41	1.92	10	1
1:A:1785:ASN:ND2	1:A:1788:GLN:HB3	0.41	2.30	13	1
1:A:1716:LEU:CD2	1:A:1775:LEU:HD11	0.41	2.46	14	1
1:A:1764:GLN:OE1	1:A:1810:LEU:HA	0.41	2.15	1	1
1:A:1714:GLU:N	1:A:1715:PRO:HD2	0.41	2.30	6	1
1:A:1752:THR:HB	1:A:1758:GLN:CB	0.41	2.44	10	1
1:A:1749:ALA:HA	1:A:1758:GLN:HG2	0.41	1.92	13	1
1:A:1752:THR:HG23	1:A:1821:ALA:HB1	0.41	1.92	20	1
1:A:1798:GLU:O	1:A:1802:MET:HB2	0.41	2.15	11	1
1:A:1817:ALA:O	1:A:1821:ALA:HB3	0.41	2.15	11	1
1:A:1690:ARG:HD2	1:A:1690:ARG:C	0.41	2.41	7	1
1:A:1798:GLU:O	1:A:1802:MET:HG3	0.41	2.16	18	1
1:A:1753:LEU:O	1:A:1753:LEU:HD23	0.41	2.16	19	1
1:A:1716:LEU:HG	1:A:1730:LYS:HB2	0.41	1.93	20	1
1:A:1752:THR:CG2	1:A:1821:ALA:HB1	0.41	2.46	7	1
1:A:1793:GLN:O	1:A:1797:GLU:HG2	0.40	2.16	1	1
1:A:1668:LEU:HD23	1:A:1773:LEU:HA	0.40	1.92	2	1
1:A:1775:LEU:HD13	1:A:1775:LEU:C	0.40	2.42	14	1
1:A:1719:ALA:O	1:A:1723:GLU:N	0.40	2.54	6	1
1:A:1704:THR:O	1:A:1708:GLU:HG2	0.40	2.15	13	1
1:A:1690:ARG:NE	1:A:1693:ILE:HG22	0.40	2.31	19	1
1:A:1661:CYS:HB2	1:A:1780:LYS:HG3	0.40	1.94	10	1
1:A:1698:LEU:HD12	1:A:1751:LYS:NZ	0.40	2.31	16	1
1:A:1679:SER:O	1:A:1683:VAL:HG23	0.40	2.17	3	1
1:A:1785:ASN:ND2	1:A:1788:GLN:H	0.40	2.14	17	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	163/174 (94%)	156±2 (96±1%)	5±2 (3±1%)	2±1 (1±1%)	13	61
All	All	3260/3480 (94%)	3116 (96%)	106 (3%)	38 (1%)	13	61

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	1783	GLY	18
1	A	1692	GLY	9
1	A	1790	ALA	5
1	A	1690	ARG	3
1	A	1691	GLU	2
1	A	1789	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	124/132 (94%)	120±2 (97±1%)	4±2 (3±1%)	34	83
All	All	2480/2640 (94%)	2399 (97%)	81 (3%)	34	83

All 29 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	1690	ARG	7
1	A	1658	GLN	6
1	A	1691	GLU	5
1	A	1696	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	1712	LEU	5
1	A	1741	LEU	5
1	A	1796	LEU	5
1	A	1687	LEU	4
1	A	1758	GLN	4
1	A	1751	LYS	4
1	A	1672	LEU	3
1	A	1723	GLU	3
1	A	1736	GLN	3
1	A	1785	ASN	3
1	A	1727	LEU	2
1	A	1788	GLN	2
1	A	1677	GLN	2
1	A	1703	LEU	2
1	A	1761	LEU	1
1	A	1775	LEU	1
1	A	1774	GLN	1
1	A	1781	GLU	1
1	A	1802	MET	1
1	A	1757	GLN	1
1	A	1787	LYS	1
1	A	1726	GLN	1
1	A	1699	HIS	1
1	A	1780	LYS	1
1	A	1815	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides 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