



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 09:17 AM EST

PDB ID : 2KE7
Title : NMR structure of the first SAM domain from AIDA1
Authors : Donaldson, L.
Deposited on : 2009-01-27

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.27
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

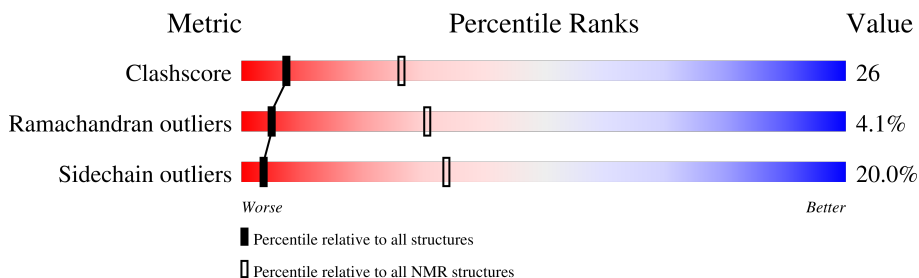
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	103	

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 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:815-A:875 (61)	0.55	10

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 7, 9, 10
2	3, 6
Single-model clusters	8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 908 atoms, of which 407 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ankyrin repeat and sterile alpha motif domain-containing protein 1B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	63	908	315	407	88	95	3	0

There are 17 discrepancies between the modelled and reference sequences:

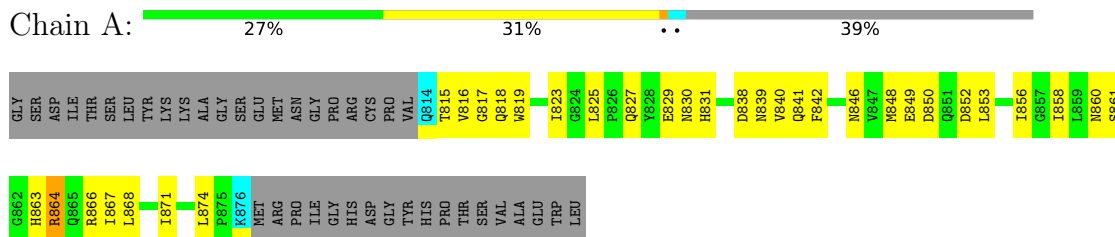
Chain	Residue	Modelled	Actual	Comment	Reference
A	792	GLY	-	expression tag	UNP Q7Z6G8
A	793	SER	-	expression tag	UNP Q7Z6G8
A	794	ASP	-	expression tag	UNP Q7Z6G8
A	795	ILE	-	expression tag	UNP Q7Z6G8
A	796	THR	-	expression tag	UNP Q7Z6G8
A	797	SER	-	expression tag	UNP Q7Z6G8
A	798	LEU	-	expression tag	UNP Q7Z6G8
A	799	TYR	-	expression tag	UNP Q7Z6G8
A	800	LYS	-	expression tag	UNP Q7Z6G8
A	801	LYS	-	expression tag	UNP Q7Z6G8
A	802	ALA	-	expression tag	UNP Q7Z6G8
A	803	GLY	-	expression tag	UNP Q7Z6G8
A	804	SER	-	expression tag	UNP Q7Z6G8
A	805	GLU	-	expression tag	UNP Q7Z6G8
A	806	MET	-	expression tag	UNP Q7Z6G8
A	807	ASN	-	expression tag	UNP Q7Z6G8
A	808	GLY	-	expression tag	UNP Q7Z6G8

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: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

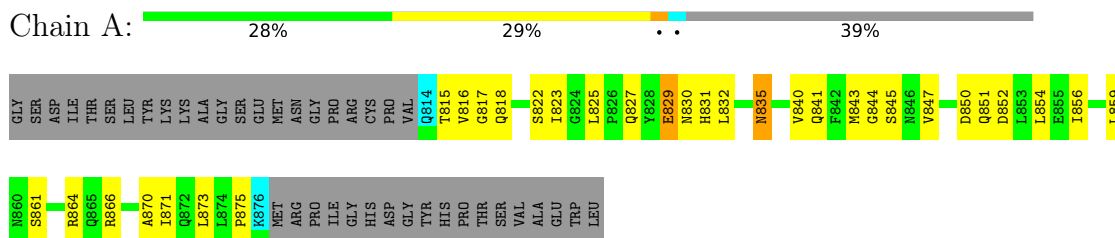


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

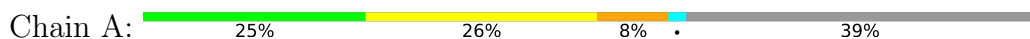
4.2.1 Score per residue for model 1

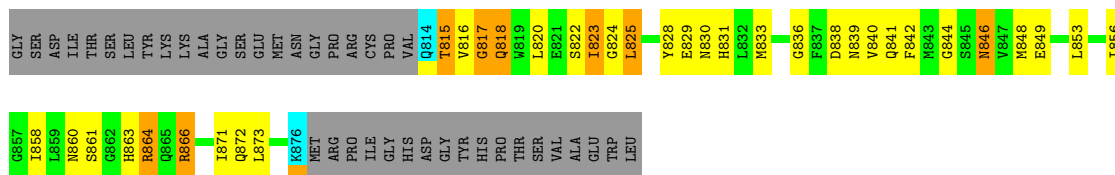
- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B



4.2.2 Score per residue for model 2

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

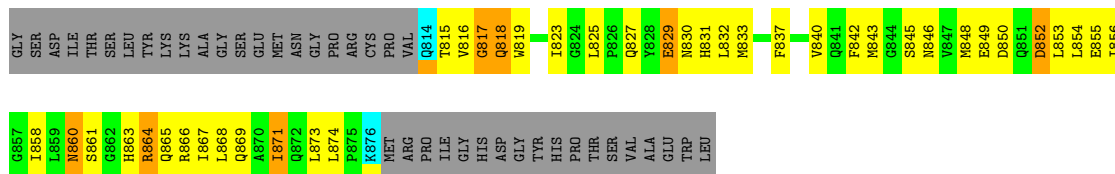




4.2.3 Score per residue for model 3

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

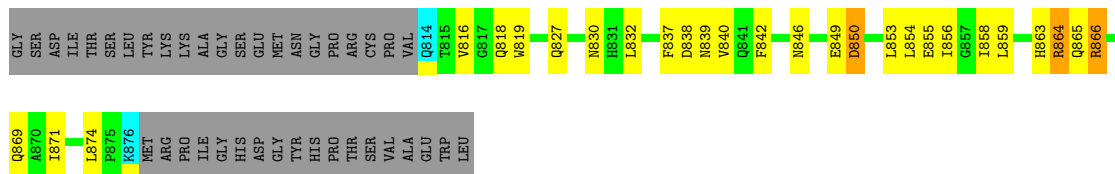
Chain A: 20% 32% 7% 39%



4.2.4 Score per residue for model 4

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

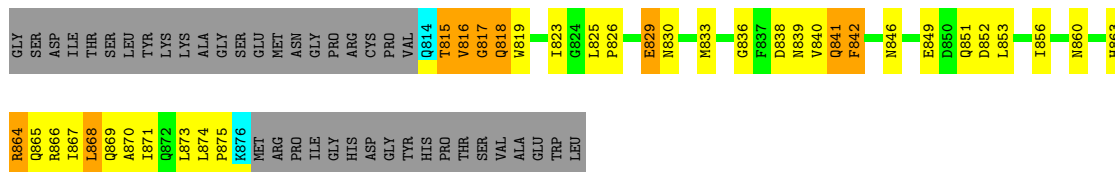
Chain A: 33% 23% 7% 39%



4.2.5 Score per residue for model 5

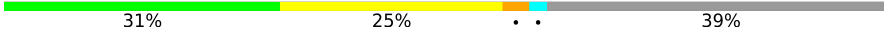
- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

Chain A: 24% 26% 9% 39%



4.2.6 Score per residue for model 6

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

Chain A: 

GLY SER ASP ILE THR SER LEU TYR LYS ALA ASP GLY SER MET ASN PRO ARG CYS PRO VAL Q814 G817 Q818 W819 L820 I823 G824 L825 P826 Q827 Y828 D838 N839 V840 Q841 F842 N846 E849 D850 L853 I856 N860 S861 G862 H863 R864 Q865 R866 I867 L868

Q869 A870 R876 MET ARG PRO ILE GLY HIS ASP GLY SER THR HIS PRO MET THR SER VAL ALA GLU TRP LEU

4.2.7 Score per residue for model 7

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

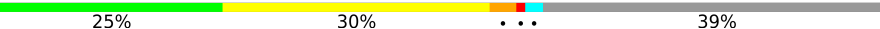
Chain A: 

GLY SER ASP THR SER LEU TYR LYS ALA GLY SER MET ASN PRO ARG CYS VAL I815 W816 G817 W819 L820 I823 G824 L825 Q827 Y828 E829 H830 H831 L832 F837 D838 N839 W840 Q841 F842 S845 I846 W847 N848 E849 E849 D850 Q851 D852 L853 L854 E855 E856

I868 L869 N860 S861 G862 H863 R864 Q865 R866 L867 L868 I871 Q872 L874 R875 K876 MET ARG PRO ILE HIS ASP GLY TYR HIS PRO THR SER VAL I815 W816 G817 W819 L820 I823 G824 L825 Q827 Y828 E829 H830 H831 L832 F837 D838 N839 W840 Q841 F842 S845 I846 W847 N848 E849 E849 D850 Q851 D852 L853 L854 E855 E856

4.2.8 Score per residue for model 8

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B


Chain A: 

GLY SER ASP THR SER LEU TYR LYS ALA GLY SER MET ASN PRO ARG CYS VAL Q814 W816 G817 W819 I823 G824 L825 P826 Q827 H830 H831 M835 G836 F837 D838 N839 Q841 F842 N846 V847 M848 E849 D850 D852 L853 L854 E855 I856 I858

L869 N860 S861 G862 H863 R864 Q865 R866 I871 L874 R875 K876 MET ARG PRO ILE GLY SER THR HIS PRO THR SER VAL ALA GLU TRP LEU

4.2.9 Score per residue for model 9

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

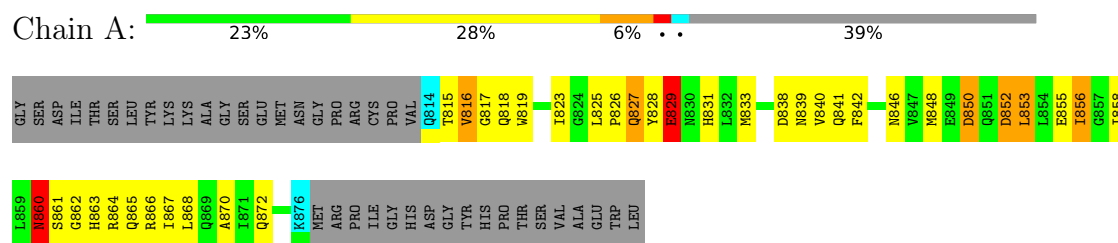
Chain A: 

GLY SER ASP ILE THR SER LEU TYR LYS ALA GLY SER MET ASN PRO ARG CYS PRO VAL Q814 W816 G817 I823 E829 N830 H831 F837 D838 N839 V840 Q841 F842 M843 G844 S845 N846 W847 M848 E849 D850 Q851 D852 L853 I856 G857 I858 L859 N860 S861 R864 Q865

R866 I867 L868 Q869 A870 I871 Q872 L873 L874 R875 K876 MET ARG PRO ILE GLY HIS ASP GLY TYR HIS PRO MET THR SER VAL ALA GLU TRP LEU

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing*.

Of the 25 calculated structures, 10 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
X-PLOR NIH	refinement	2.21
CYANA	structure solution	2.1

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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 i

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	483	398	471	25±6
All	All	4830	3980	4710	249

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:823:ILE:HG21	1:A:870:ALA:HB2	0.93	1.38	5	2
1:A:819:TRP:CE3	1:A:840:VAL:HG11	0.85	2.06	6	3
1:A:817:GLY:H	1:A:820:LEU:HD12	0.77	1.37	6	1
1:A:853:LEU:HD13	1:A:864:ARG:CG	0.75	2.11	8	1
1:A:846:ASN:ND2	1:A:847:VAL:HG22	0.73	1.98	8	1
1:A:853:LEU:HD13	1:A:864:ARG:HG3	0.69	1.63	8	1
1:A:816:VAL:HG11	1:A:832:LEU:HD22	0.68	1.65	1	1
1:A:816:VAL:HG13	1:A:840:VAL:CG1	0.67	2.18	1	1
1:A:853:LEU:HD13	1:A:864:ARG:HB3	0.67	1.65	9	2
1:A:853:LEU:HD13	1:A:864:ARG:HA	0.66	1.65	3	1
1:A:823:ILE:HG21	1:A:870:ALA:HB1	0.66	1.66	6	2
1:A:853:LEU:HD12	1:A:864:ARG:HD2	0.65	1.68	5	2
1:A:846:ASN:HD21	1:A:847:VAL:HG22	0.65	1.52	8	1
1:A:820:LEU:HD13	1:A:828:TYR:CB	0.65	2.22	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:853:LEU:HD23	1:A:858:ILE:HB	0.64	1.68	10	1
1:A:825:LEU:N	1:A:825:LEU:HD13	0.64	2.08	2	1
1:A:848:MET:N	1:A:848:MET:SD	0.64	2.71	9	1
1:A:825:LEU:N	1:A:826:PRO:CD	0.60	2.65	10	2
1:A:842:PHE:O	1:A:846:ASN:N	0.59	2.35	9	8
1:A:820:LEU:HD13	1:A:828:TYR:HB3	0.59	1.74	7	1
1:A:823:ILE:O	1:A:866:ARG:NH1	0.59	2.36	2	2
1:A:860:ASN:O	1:A:863:HIS:CD2	0.59	2.55	5	2
1:A:853:LEU:HD22	1:A:864:ARG:HA	0.59	1.74	10	1
1:A:831:HIS:NE2	1:A:856:ILE:O	0.58	2.36	10	2
1:A:853:LEU:HD13	1:A:864:ARG:HD2	0.57	1.76	10	1
1:A:852:ASP:OD1	1:A:853:LEU:N	0.57	2.36	5	1
1:A:828:TYR:CZ	1:A:867:ILE:HG13	0.57	2.34	7	1
1:A:868:LEU:HD12	1:A:868:LEU:C	0.57	2.20	5	2
1:A:850:ASP:HA	1:A:853:LEU:HD12	0.56	1.77	7	2
1:A:829:GLU:H	1:A:829:GLU:CD	0.56	2.04	1	2
1:A:863:HIS:CD2	1:A:864:ARG:H	0.56	2.17	5	2
1:A:853:LEU:HD21	1:A:867:ILE:HG13	0.56	1.76	5	3
1:A:825:LEU:HD11	1:A:866:ARG:CB	0.56	2.31	8	2
1:A:860:ASN:O	1:A:863:HIS:ND1	0.55	2.33	3	1
1:A:824:GLY:C	1:A:825:LEU:HD13	0.55	2.21	2	1
1:A:823:ILE:HG21	1:A:870:ALA:CB	0.55	2.24	5	4
1:A:860:ASN:O	1:A:863:HIS:NE2	0.55	2.40	5	2
1:A:852:ASP:CG	1:A:853:LEU:N	0.55	2.60	10	1
1:A:823:ILE:CD1	1:A:825:LEU:HD12	0.54	2.33	3	2
1:A:841:GLN:H	1:A:841:GLN:CD	0.54	2.06	6	1
1:A:848:MET:SD	1:A:872:GLN:HG2	0.53	2.42	10	1
1:A:828:TYR:CE2	1:A:858:ILE:HD12	0.53	2.39	2	1
1:A:861:SER:HA	1:A:864:ARG:NH1	0.53	2.18	1	1
1:A:823:ILE:HD12	1:A:825:LEU:HD12	0.53	1.81	3	2
1:A:858:ILE:HG21	1:A:864:ARG:N	0.53	2.19	4	1
1:A:819:TRP:CE2	1:A:874:LEU:HD11	0.53	2.39	8	1
1:A:853:LEU:HD13	1:A:864:ARG:HG2	0.53	1.81	8	1
1:A:815:THR:O	1:A:817:GLY:N	0.52	2.42	5	3
1:A:823:ILE:O	1:A:866:ARG:NH2	0.52	2.36	3	3
1:A:863:HIS:CG	1:A:864:ARG:N	0.52	2.77	3	3
1:A:817:GLY:N	1:A:820:LEU:HD12	0.52	2.15	6	1
1:A:825:LEU:HD11	1:A:866:ARG:HB3	0.52	1.80	8	1
1:A:840:VAL:HA	1:A:843:MET:SD	0.52	2.44	9	1
1:A:838:ASP:O	1:A:839:ASN:CB	0.52	2.58	7	1
1:A:835:ASN:ND2	1:A:837:PHE:CE1	0.51	2.79	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:830:ASN:OD1	1:A:831:HIS:N	0.51	2.42	9	2
1:A:868:LEU:HG	1:A:869:GLN:N	0.51	2.21	5	1
1:A:858:ILE:HG21	1:A:863:HIS:CG	0.51	2.41	3	1
1:A:853:LEU:HD13	1:A:863:HIS:ND1	0.51	2.21	5	1
1:A:861:SER:OG	1:A:864:ARG:NH1	0.50	2.35	1	1
1:A:816:VAL:HG22	1:A:838:ASP:CG	0.50	2.28	8	1
1:A:816:VAL:O	1:A:818:GLN:N	0.50	2.45	7	1
1:A:853:LEU:HD23	1:A:858:ILE:CB	0.50	2.36	10	1
1:A:866:ARG:O	1:A:870:ALA:N	0.49	2.43	1	2
1:A:841:GLN:NE2	1:A:875:PRO:O	0.49	2.44	1	1
1:A:832:LEU:HD22	1:A:843:MET:SD	0.49	2.47	3	1
1:A:825:LEU:HB3	1:A:863:HIS:CG	0.49	2.42	2	1
1:A:850:ASP:O	1:A:854:LEU:N	0.49	2.43	8	1
1:A:871:ILE:HA	1:A:874:LEU:HD12	0.48	1.85	4	3
1:A:819:TRP:CD2	1:A:840:VAL:HG11	0.48	2.44	7	3
1:A:853:LEU:CD1	1:A:864:ARG:HA	0.48	2.38	6	2
1:A:838:ASP:O	1:A:839:ASN:C	0.48	2.52	4	1
1:A:852:ASP:OD1	1:A:864:ARG:NH1	0.48	2.46	5	1
1:A:819:TRP:CE2	1:A:870:ALA:HB1	0.48	2.43	5	1
1:A:829:GLU:CD	1:A:829:GLU:N	0.48	2.67	1	2
1:A:869:GLN:HG3	1:A:870:ALA:N	0.48	2.24	9	1
1:A:823:ILE:CG1	1:A:825:LEU:HD12	0.47	2.40	3	1
1:A:839:ASN:ND2	1:A:842:PHE:CG	0.47	2.83	8	1
1:A:841:GLN:HA	1:A:874:LEU:HD13	0.47	1.86	5	1
1:A:864:ARG:HB3	1:A:864:ARG:CZ	0.47	2.40	6	1
1:A:860:ASN:ND2	1:A:863:HIS:CE1	0.47	2.82	7	1
1:A:838:ASP:CG	1:A:839:ASN:N	0.47	2.68	10	3
1:A:830:ASN:OD1	1:A:831:HIS:ND1	0.47	2.45	2	1
1:A:840:VAL:HG23	1:A:841:GLN:N	0.47	2.25	5	2
1:A:849:GLU:N	1:A:852:ASP:OD2	0.47	2.48	3	1
1:A:860:ASN:OD1	1:A:860:ASN:N	0.46	2.46	7	1
1:A:858:ILE:O	1:A:864:ARG:NH1	0.46	2.48	8	1
1:A:860:ASN:OD1	1:A:863:HIS:ND1	0.46	2.39	8	1
1:A:818:GLN:N	1:A:818:GLN:OE1	0.46	2.42	7	1
1:A:826:PRO:O	1:A:827:GLN:CB	0.46	2.64	8	3
1:A:852:ASP:OD2	1:A:853:LEU:HD12	0.46	2.10	10	1
1:A:816:VAL:HG12	1:A:840:VAL:CG1	0.46	2.41	7	1
1:A:850:ASP:OD1	1:A:864:ARG:NH1	0.46	2.43	7	1
1:A:828:TYR:CD1	1:A:858:ILE:HD12	0.46	2.45	10	1
1:A:863:HIS:CD2	1:A:864:ARG:N	0.45	2.84	5	1
1:A:826:PRO:O	1:A:827:GLN:HB3	0.45	2.12	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:827:GLN:O	1:A:831:HIS:ND1	0.45	2.40	1	3
1:A:819:TRP:CD1	1:A:874:LEU:HD21	0.45	2.46	5	1
1:A:818:GLN:O	1:A:822:SER:N	0.45	2.39	1	2
1:A:828:TYR:OH	1:A:858:ILE:CG2	0.45	2.65	2	1
1:A:860:ASN:HD21	1:A:863:HIS:CE1	0.45	2.29	7	1
1:A:846:ASN:C	1:A:846:ASN:HD22	0.45	2.15	2	1
1:A:820:LEU:HD22	1:A:828:TYR:CB	0.45	2.42	2	1
1:A:828:TYR:OH	1:A:858:ILE:HG21	0.45	2.11	7	1
1:A:866:ARG:NH2	1:A:869:GLN:OE1	0.45	2.41	6	2
1:A:848:MET:SD	1:A:872:GLN:NE2	0.44	2.89	7	1
1:A:828:TYR:CE1	1:A:858:ILE:HD12	0.44	2.46	10	1
1:A:820:LEU:HD22	1:A:828:TYR:HB3	0.44	1.89	7	1
1:A:849:GLU:O	1:A:852:ASP:CG	0.44	2.56	5	1
1:A:842:PHE:CD2	1:A:846:ASN:ND2	0.44	2.86	3	1
1:A:816:VAL:HG21	1:A:833:MET:HG3	0.44	1.89	10	2
1:A:871:ILE:O	1:A:875:PRO:CD	0.44	2.66	5	1
1:A:861:SER:OG	1:A:864:ARG:NH2	0.44	2.34	7	2
1:A:825:LEU:HD11	1:A:866:ARG:HB2	0.44	1.88	7	1
1:A:835:ASN:O	1:A:835:ASN:ND2	0.44	2.41	1	1
1:A:823:ILE:HB	1:A:825:LEU:HD11	0.44	1.89	2	1
1:A:852:ASP:OD2	1:A:864:ARG:NH1	0.44	2.48	5	1
1:A:823:ILE:O	1:A:866:ARG:NE	0.44	2.38	9	1
1:A:825:LEU:N	1:A:826:PRO:HD3	0.44	2.27	10	1
1:A:874:LEU:N	1:A:875:PRO:CD	0.43	2.81	9	1
1:A:825:LEU:HD11	1:A:866:ARG:HD2	0.43	1.89	10	1
1:A:829:GLU:CG	1:A:830:ASN:N	0.43	2.81	1	2
1:A:840:VAL:C	1:A:874:LEU:HD13	0.43	2.34	5	1
1:A:850:ASP:OD1	1:A:864:ARG:NH2	0.43	2.47	4	2
1:A:865:GLN:NE2	1:A:869:GLN:OE1	0.43	2.47	4	1
1:A:850:ASP:HA	1:A:864:ARG:CD	0.43	2.43	3	2
1:A:867:ILE:O	1:A:871:ILE:HG12	0.43	2.14	3	1
1:A:865:GLN:HA	1:A:868:LEU:HD23	0.43	1.91	5	1
1:A:819:TRP:CZ2	1:A:870:ALA:CB	0.43	3.02	6	1
1:A:819:TRP:CZ2	1:A:870:ALA:HB1	0.43	2.49	6	1
1:A:866:ARG:NE	1:A:869:GLN:OE1	0.43	2.46	5	1
1:A:826:PRO:O	1:A:827:GLN:NE2	0.43	2.51	10	1
1:A:850:ASP:OD1	1:A:864:ARG:NE	0.43	2.46	1	1
1:A:816:VAL:HG11	1:A:832:LEU:CD2	0.43	2.44	7	1
1:A:853:LEU:HD11	1:A:868:LEU:HD11	0.43	1.89	9	1
1:A:818:GLN:O	1:A:822:SER:OG	0.43	2.35	2	1
1:A:858:ILE:HG23	1:A:863:HIS:CB	0.43	2.44	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:865:GLN:OE1	1:A:866:ARG:NE	0.43	2.39	4	1
1:A:862:GLY:O	1:A:863:HIS:C	0.42	2.57	6	1
1:A:853:LEU:HD11	1:A:867:ILE:HB	0.42	1.91	10	1
1:A:844:GLY:HA2	1:A:871:ILE:HG23	0.42	1.92	9	1
1:A:871:ILE:O	1:A:875:PRO:HD3	0.42	2.14	5	1
1:A:841:GLN:NE2	1:A:845:SER:OG	0.42	2.52	7	1
1:A:862:GLY:O	1:A:865:GLN:NE2	0.42	2.43	10	1
1:A:819:TRP:CE3	1:A:840:VAL:CG1	0.42	3.03	3	2
1:A:871:ILE:HG22	1:A:874:LEU:HD12	0.42	1.91	3	1
1:A:825:LEU:HD21	1:A:866:ARG:CZ	0.42	2.44	1	1
1:A:851:GLN:O	1:A:855:GLU:N	0.42	2.51	8	2
1:A:825:LEU:HD13	1:A:867:ILE:HG12	0.42	1.90	8	1
1:A:864:ARG:NH1	1:A:864:ARG:O	0.42	2.52	10	1
1:A:839:ASN:C	1:A:839:ASN:OD1	0.42	2.58	4	1
1:A:816:VAL:HG23	1:A:817:GLY:N	0.42	2.29	7	1
1:A:850:ASP:OD2	1:A:864:ARG:NH2	0.42	2.51	10	1
1:A:861:SER:CA	1:A:864:ARG:NH1	0.42	2.83	1	1
1:A:868:LEU:CG	1:A:869:GLN:N	0.42	2.83	5	2
1:A:864:ARG:HB3	1:A:864:ARG:NH1	0.42	2.30	6	1
1:A:846:ASN:CG	1:A:847:VAL:N	0.42	2.72	8	1
1:A:832:LEU:HG	1:A:837:PHE:CG	0.42	2.49	4	1
1:A:853:LEU:O	1:A:856:ILE:HG13	0.41	2.15	4	1
1:A:868:LEU:C	1:A:868:LEU:CD1	0.41	2.86	5	1
1:A:825:LEU:N	1:A:825:LEU:CD1	0.41	2.80	2	1
1:A:832:LEU:HG	1:A:837:PHE:CD2	0.41	2.50	4	1
1:A:843:MET:O	1:A:847:VAL:N	0.41	2.53	1	1
1:A:866:ARG:NH1	1:A:869:GLN:OE1	0.41	2.40	9	1
1:A:827:GLN:N	1:A:829:GLU:OE1	0.41	2.48	10	1
1:A:829:GLU:HG2	1:A:830:ASN:N	0.41	2.30	3	2
1:A:848:MET:HB3	1:A:871:ILE:HD12	0.41	1.93	3	1
1:A:863:HIS:O	1:A:867:ILE:CG1	0.41	2.68	3	1
1:A:819:TRP:CG	1:A:840:VAL:HG11	0.41	2.50	4	1
1:A:874:LEU:HB2	1:A:875:PRO:HD3	0.41	1.91	5	1
1:A:820:LEU:HD13	1:A:828:TYR:HB2	0.41	1.92	6	1
1:A:860:ASN:ND2	1:A:863:HIS:CG	0.41	2.89	7	1
1:A:825:LEU:HB3	1:A:863:HIS:CD2	0.41	2.51	2	1
1:A:850:ASP:CG	1:A:864:ARG:NH2	0.41	2.73	10	1
1:A:844:GLY:HA2	1:A:871:ILE:HB	0.41	1.93	1	1
1:A:844:GLY:CA	1:A:871:ILE:HB	0.41	2.46	2	1
1:A:868:LEU:HD12	1:A:869:GLN:N	0.41	2.31	3	1
1:A:858:ILE:HG23	1:A:863:HIS:HB3	0.41	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:838:ASP:OD1	1:A:839:ASN:N	0.41	2.50	6	1
1:A:825:LEU:HD23	1:A:825:LEU:HA	0.41	1.78	7	1
1:A:825:LEU:CD2	1:A:825:LEU:O	0.40	2.70	2	1
1:A:833:MET:O	1:A:836:GLY:N	0.40	2.54	2	1
1:A:860:ASN:OD1	1:A:860:ASN:C	0.40	2.59	3	1
1:A:836:GLY:O	1:A:838:ASP:N	0.40	2.52	5	1
1:A:860:ASN:HB3	1:A:863:HIS:CG	0.40	2.51	10	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	61/103 (59%)	52±1 (85±2%)	7±1 (11±2%)	2±1 (4±2%)	5	31
All	All	610/1030 (59%)	519 (85%)	66 (11%)	25 (4%)	5	31

All 10 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	817	GLY	8
1	A	816	VAL	5
1	A	860	ASN	3
1	A	829	GLU	2
1	A	827	GLN	2
1	A	859	LEU	1
1	A	849	GLU	1
1	A	839	ASN	1
1	A	858	ILE	1
1	A	875	PRO	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	53/88 (60%)	42±3 (80±5%)	11±3 (20±5%)	4	34
All	All	530/880 (60%)	424 (80%)	106 (20%)	4	34

All 36 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	856	ILE	8
1	A	815	THR	6
1	A	829	GLU	6
1	A	852	ASP	5
1	A	873	LEU	5
1	A	861	SER	5
1	A	864	ARG	5
1	A	854	LEU	4
1	A	818	GLN	4
1	A	849	GLU	4
1	A	830	ASN	4
1	A	841	GLN	4
1	A	868	LEU	4
1	A	848	MET	3
1	A	837	PHE	3
1	A	855	GLU	3
1	A	827	GLN	3
1	A	850	ASP	3
1	A	845	SER	2
1	A	851	GLN	2
1	A	859	LEU	2
1	A	846	ASN	2
1	A	866	ARG	2
1	A	865	GLN	2
1	A	871	ILE	2
1	A	816	VAL	2
1	A	860	ASN	2
1	A	835	ASN	1
1	A	823	ILE	1
1	A	825	LEU	1
1	A	833	MET	1
1	A	842	PHE	1
1	A	828	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	863	HIS	1
1	A	838	ASP	1
1	A	853	LEU	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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided