



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:26 pm BST

PDB ID : 2KBT
Title : Attachment of an NMR-invisible solubility enhancement tag (INSET) using a sortase-mediated protein ligation method
Authors : Kumeta, H.; Kobashigawa, Y.; Ogura, K.; Inagaki, F.
Deposited on : 2008-12-07

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

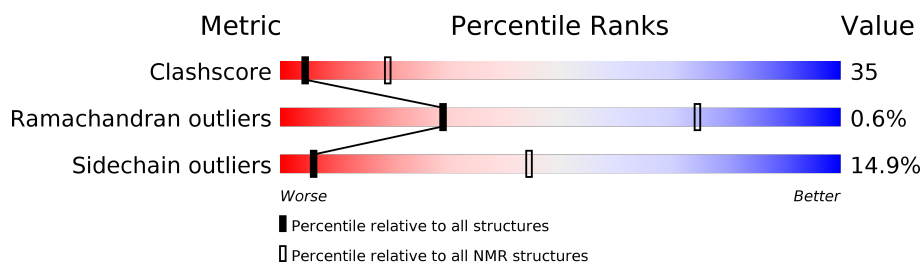
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	142	

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:785-A:814, A:819-A:841 (53)	0.24	15

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

3 Entry composition

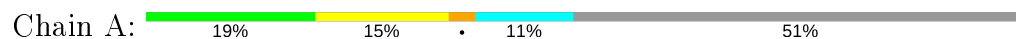
There is only 1 type of molecule in this entry. The entry contains 1102 atoms, of which 536 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms						Trace
1	A	69	Total	C	H	N	O	S	0
			1102	362	536	96	107	1	

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	GLY	-	expression tag	UNP P27870
A	781	PRO	-	expression tag	UNP P27870
A	782	GLY	-	expression tag	UNP P27870
A	783	THR	-	expression tag	UNP P27870
A	845	LEU	-	linker	UNP P27870
A	846	PRO	-	linker	UNP P27870
A	847	GLU	-	linker	UNP P27870
A	848	THR	-	linker	UNP P27870
A	849	GLY	-	linker	UNP P27870
A	850	GLY	-	linker	UNP P27870
A	851	GLY	-	linker	UNP P27870
A	852	SER	-	linker	UNP P27870
A	853	GLY	-	linker	UNP P27870
A	854	SER	-	linker	UNP P27870
A	855	SER	-	linker	UNP P27870
A	856	MET	-	expression tag	UNP P06654
A	912	HIS	-	expression tag	UNP P06654
A	913	SER	-	expression tag	UNP P06654
A	914	LEU	-	expression tag	UNP P06654
A	915	GLU	-	expression tag	UNP P06654
A	916	HIS	-	expression tag	UNP P06654
A	917	HIS	-	expression tag	UNP P06654
A	918	HIS	-	expression tag	UNP P06654
A	919	HIS	-	expression tag	UNP P06654
A	920	HIS	-	expression tag	UNP P06654
A	921	HIS	-	expression tag	UNP P06654






SER GLY SER SER MET THR THR LYS LEU LEU LEU ASN GLY LYS THR LYS GLY GLU THR THR THR ALA VAL ASP ALA ALA THR ALA GLU LYS VAL PHE LYS GLN TYR ALA ASN ASP ASN GLY VAL ASP GLY GLU TRP THR THR ASP ASP ALA THR LYS PHE THR VAL THR GLU

HIS
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HIS

4.2.12 Score per residue for model 12

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G

Chain A: 


G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 R796 R797 R798 L801 S802 L803 K804 I808 I809 K810 K811 K814 K815 K816 K817 Q818 Q819 W820 W821 E824 I825 Y826 I829 G830 W831 F832 F833 S834 V837 E838 E839 E840 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY

GLY GLY SER GLY SER SER MET THR TYR THR LYS LEU LEU ILE LEU ASN GLY LYS THR LYS LEU GLY LYS THR I808 I809 K810 K811 K814 K815 K816 K817 Q818 Q819 W820 W821 E824 I825 Y826 I829 G830 W831 F832 F833 S834 V837 E838 E839 E840 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY

THR
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4.2.13 Score per residue for model 13

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G

Chain A: 


G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 R796 R801 S802 I808 I809 L812 N813 K814 K815 K816 K817 Q818 Q819 W820 W821 R822 G823 E824 I825 Y826 I829 G830 W831 F832 F833 V837 E838 E839 E840 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY GLY GLY MET

THR THR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY GLU THR THR THR ALA VAL ASP ALA ALA THR THR I808 I809 L812 N813 K814 K815 K816 K817 Q818 Q819 W820 W821 R822 G823 E824 I825 Y826 I829 G830 W831 F832 F833 V837 E838 E839 E840 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY GLY GLY MET

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4.2.14 Score per residue for model 14

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G

Chain A: 


G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 R796 R801 S802 L803 K804 I808 I809 L812 N813 K814 K815 K816 K817 Q818 Q819 W820 W821 R822 G823 E824 I825 Y826 I829 G830 W831 F832 F833 S834 V837 E838 E839 E840 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY GLY GLY MET

SER SER MET THR THR LYS LEU LEU ILE LEU ASN GLY LYS THR LYS LEU GLY GLY GLU THR THR THR ALA VAL ASP ALA ALA THR THR I808 I809 L812 N813 K814 K815 K816 K817 Q818 Q819 W820 W821 R822 G823 E824 I825 Y826 I829 G830 W831 F832 F833 S834 V837 E838 E839 E840 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY GLY GLY MET

LEU
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4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G

Chain A: 


G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G796 G798 L801 L802 L803 L804 L805 L808 L809 K810 K811 K814 K815 Q816 Q817 Q818 Q819 W820 W821 E824 E825 I829 G830 W831 F832 F833 S834 V837 E838 E839 D840 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY

SER GLY SER SER MET THR TYR LYS LEU ILE LEU ASN GLY LYS THR L801 L802 L803 L804 L805 L808 L809 VAL ASP ALA ALA THR ALA GLU LYS VAL PHE LYS GLN TYR ALA ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ASP ALA THR LYS PHE VAL THR VAL GLU

HIS
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4.2.16 Score per residue for model 16

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G

Chain A: 


G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G796 G801 G802 L803 L808 L809 L812 K814 K815 Q816 Q817 Q818 Q819 W820 W821 E824 E825 I829 G830 W831 F832 F833 S834 V837 E838 E839 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY GLY

SER SER MET THR TYR LYS LEU ILE LEU ASN GLY LYS THR L801 L802 L803 L808 L809 VAL ASP ALA ALA THR ALA GLU LYS VAL PHE LYS GLN TYR ALA ASN ASP ASN GLY VAL ASP GLY GLY TRP THR TYR ASP ASP ALA THR LYS PHE VAL THR VAL THR GLU HIS SER

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4.2.17 Score per residue for model 17

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G

Chain A: 

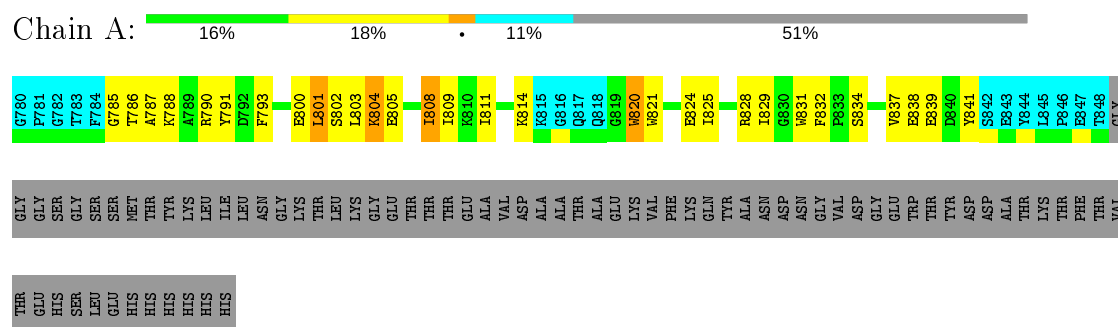
G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 E800 E801 S802 L803 L804 L808 L809 L812 K815 Q816 Q817 Q818 Q819 W820 W821 E824 E825 I829 G830 W831 F832 F833 S834 N835 V836 V837 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY SER SER GLY SER

MET THR TYR LYS LEU ILE LEU ASN GLY LYS THR L801 L802 L803 L804 L808 L809 VAL ASP ALA ALA THR ALA GLU LYS VAL PHE LYS GLN TYR E824 E825 I829 G830 W831 F832 F833 S834 N835 V836 V837 Y841 S842 E843 Y844 L845 P846 E847 T848 GLY GLY GLY SER SER GLY SER

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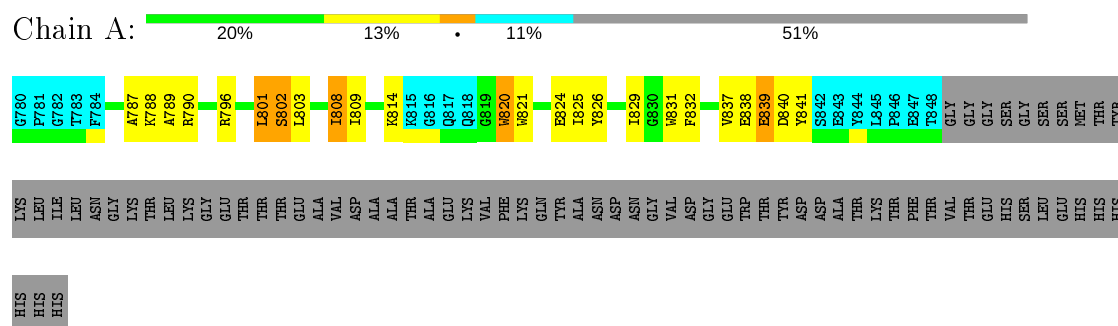
4.2.18 Score per residue for model 18

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G



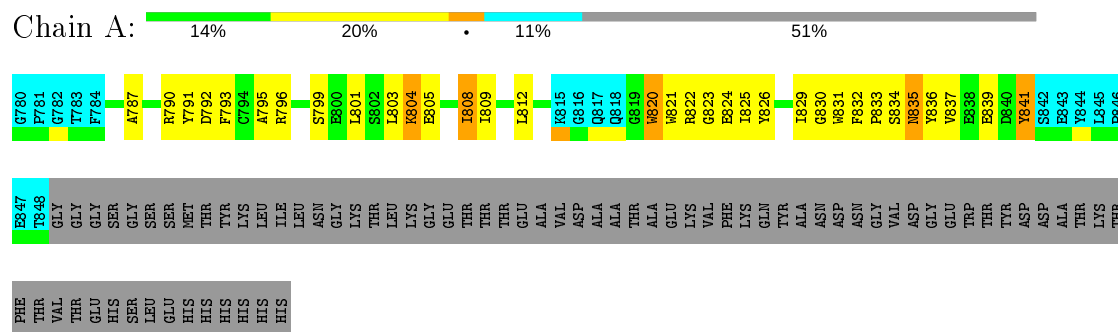
4.2.19 Score per residue for model 19

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G



4.2.20 Score per residue for model 20

- Molecule 1: chimera of Proto-oncogene vav, linker, Immunoglobulin G-binding protein G



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, distance geometry*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Sparky	refinement	3.110
CYANA	structure solution	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	862
Number of shifts mapped to atoms	862
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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	444	423	423	30±6
All	All	8880	8460	8460	606

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:811:ILE:HG21	1:A:814:LYS:NZ	0.90	1.80	7	1
1:A:809:ILE:HG21	1:A:832:PHE:CZ	0.87	2.04	3	20
1:A:824:GLU:HB2	1:A:829:ILE:HD13	0.76	1.58	12	17
1:A:820:TRP:CE2	1:A:831:TRP:CE3	0.74	2.75	16	17
1:A:824:GLU:HB3	1:A:829:ILE:HD13	0.71	1.62	17	3
1:A:808:ILE:N	1:A:808:ILE:HD13	0.71	2.01	10	14
1:A:808:ILE:HD13	1:A:808:ILE:N	0.70	2.01	7	6
1:A:803:LEU:HD11	1:A:809:ILE:HG12	0.68	1.64	3	7
1:A:811:ILE:HG21	1:A:814:LYS:HZ1	0.68	1.49	7	1
1:A:812:LEU:CB	1:A:822:ARG:HH21	0.67	2.01	14	1
1:A:787:ALA:HB2	1:A:811:ILE:HD11	0.67	1.67	12	9
1:A:809:ILE:CG2	1:A:832:PHE:CZ	0.66	2.78	12	20
1:A:832:PHE:CE2	1:A:837:VAL:HG21	0.63	2.29	10	17
1:A:803:LEU:HD21	1:A:837:VAL:CG1	0.63	2.24	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:785:GLY:O	1:A:786:THR:HG23	0.63	1.93	10	11
1:A:832:PHE:HE2	1:A:837:VAL:HG21	0.62	1.55	12	18
1:A:809:ILE:HG21	1:A:832:PHE:CE1	0.61	2.30	15	18
1:A:808:ILE:O	1:A:825:ILE:HD11	0.61	1.96	9	9
1:A:787:ALA:CB	1:A:811:ILE:HD11	0.60	2.25	18	5
1:A:820:TRP:NE1	1:A:831:TRP:CE3	0.60	2.69	15	14
1:A:832:PHE:CD2	1:A:837:VAL:HG11	0.60	2.32	15	5
1:A:821:TRP:O	1:A:832:PHE:CD1	0.60	2.55	13	9
1:A:790:ARG:C	1:A:791:TYR:CD1	0.60	2.75	14	9
1:A:821:TRP:O	1:A:832:PHE:CE1	0.59	2.55	14	11
1:A:820:TRP:NE1	1:A:831:TRP:CZ3	0.59	2.70	4	13
1:A:824:GLU:CB	1:A:829:ILE:HD13	0.59	2.26	17	1
1:A:821:TRP:CH2	1:A:839:GLU:OE1	0.59	2.55	3	1
1:A:801:LEU:HD23	1:A:802:SER:N	0.58	2.13	17	18
1:A:834:SER:HA	1:A:837:VAL:HG22	0.57	1.75	20	5
1:A:793:PHE:CE2	1:A:800:GLU:CD	0.56	2.79	8	4
1:A:793:PHE:CE2	1:A:800:GLU:OE1	0.55	2.59	10	1
1:A:801:LEU:HD11	1:A:824:GLU:N	0.54	2.17	19	4
1:A:826:TYR:CD2	1:A:828:ARG:NH2	0.54	2.76	9	1
1:A:801:LEU:HD11	1:A:823:GLY:C	0.53	2.24	10	4
1:A:814:LYS:CD	1:A:821:TRP:CE2	0.52	2.92	8	1
1:A:826:TYR:N	1:A:826:TYR:CD1	0.52	2.75	3	7
1:A:808:ILE:CD1	1:A:808:ILE:N	0.52	2.70	16	6
1:A:811:ILE:HG21	1:A:814:LYS:HZ3	0.52	1.63	7	1
1:A:821:TRP:CZ3	1:A:834:SER:OG	0.51	2.59	12	1
1:A:812:LEU:HB2	1:A:822:ARG:HH21	0.51	1.62	14	1
1:A:820:TRP:CZ3	1:A:831:TRP:CG	0.51	2.99	10	2
1:A:814:LYS:HA	1:A:821:TRP:CD1	0.51	2.41	5	6
1:A:808:ILE:N	1:A:808:ILE:CD1	0.51	2.70	14	9
1:A:825:ILE:HG22	1:A:826:TYR:CD2	0.50	2.41	10	8
1:A:814:LYS:CD	1:A:821:TRP:CD1	0.50	2.95	7	2
1:A:824:GLU:CG	1:A:825:ILE:N	0.50	2.75	11	12
1:A:821:TRP:CH2	1:A:834:SER:OG	0.50	2.57	15	1
1:A:825:ILE:HG23	1:A:826:TYR:CE1	0.50	2.42	8	7
1:A:821:TRP:CZ3	1:A:834:SER:HB2	0.50	2.42	14	9
1:A:808:ILE:O	1:A:825:ILE:CD1	0.49	2.60	7	7
1:A:790:ARG:C	1:A:791:TYR:CG	0.49	2.86	18	9
1:A:820:TRP:CE3	1:A:831:TRP:HB3	0.49	2.42	11	14
1:A:826:TYR:CD1	1:A:826:TYR:N	0.49	2.77	9	6
1:A:793:PHE:CZ	1:A:833:PRO:HG3	0.49	2.42	20	1
1:A:785:GLY:O	1:A:786:THR:CG2	0.49	2.60	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:814:LYS:CE	1:A:821:TRP:CE2	0.49	2.96	1	1
1:A:796:ARG:CZ	1:A:797:ASP:CG	0.49	2.81	4	1
1:A:812:LEU:HB3	1:A:822:ARG:HH21	0.49	1.66	14	1
1:A:809:ILE:HG21	1:A:832:PHE:CE2	0.48	2.43	13	4
1:A:820:TRP:CE3	1:A:831:TRP:CB	0.48	2.96	10	2
1:A:821:TRP:CH2	1:A:839:GLU:OE2	0.48	2.66	12	1
1:A:825:ILE:HG23	1:A:826:TYR:CD1	0.48	2.43	3	9
1:A:801:LEU:HD23	1:A:802:SER:H	0.48	1.68	5	17
1:A:837:VAL:HG23	1:A:839:GLU:OE2	0.48	2.08	14	1
1:A:825:ILE:O	1:A:828:ARG:CD	0.48	2.61	18	1
1:A:814:LYS:HG2	1:A:821:TRP:CD1	0.48	2.44	1	3
1:A:814:LYS:NZ	1:A:821:TRP:CE3	0.48	2.81	3	1
1:A:821:TRP:CZ3	1:A:839:GLU:HG3	0.47	2.43	20	2
1:A:789:ALA:HA	1:A:837:VAL:HG12	0.47	1.84	19	1
1:A:787:ALA:HB1	1:A:838:GLU:O	0.47	2.10	16	3
1:A:790:ARG:HB2	1:A:791:TYR:CE1	0.47	2.44	16	1
1:A:793:PHE:CD2	1:A:800:GLU:OE2	0.47	2.68	6	2
1:A:814:LYS:HG3	1:A:821:TRP:CD1	0.47	2.44	7	2
1:A:824:GLU:OE1	1:A:825:ILE:CA	0.47	2.62	13	1
1:A:821:TRP:CH2	1:A:834:SER:HB2	0.46	2.45	4	5
1:A:822:ARG:HG3	1:A:831:TRP:CD1	0.46	2.46	7	2
1:A:822:ARG:NE	1:A:831:TRP:NE1	0.46	2.63	7	1
1:A:790:ARG:O	1:A:791:TYR:CG	0.46	2.69	15	6
1:A:788:LYS:HB2	1:A:841:TYR:CE2	0.46	2.46	19	5
1:A:821:TRP:CE3	1:A:834:SER:HB2	0.46	2.44	15	2
1:A:821:TRP:CH2	1:A:839:GLU:HG3	0.46	2.46	9	1
1:A:814:LYS:HD2	1:A:821:TRP:CD1	0.45	2.46	10	2
1:A:801:LEU:CB	1:A:831:TRP:O	0.45	2.65	20	1
1:A:836:TYR:O	1:A:837:VAL:CG1	0.45	2.65	14	3
1:A:793:PHE:CE2	1:A:833:PRO:HD3	0.45	2.47	20	1
1:A:803:LEU:HD11	1:A:809:ILE:CG1	0.45	2.40	3	1
1:A:788:LYS:N	1:A:838:GLU:O	0.45	2.50	18	5
1:A:787:ALA:O	1:A:809:ILE:N	0.45	2.50	7	6
1:A:825:ILE:CG2	1:A:826:TYR:CD2	0.45	3.00	10	2
1:A:839:GLU:C	1:A:841:TYR:N	0.45	2.70	7	11
1:A:790:ARG:C	1:A:791:TYR:CD2	0.45	2.90	8	2
1:A:790:ARG:NH1	1:A:790:ARG:O	0.45	2.50	7	1
1:A:824:GLU:OE2	1:A:825:ILE:CA	0.45	2.65	16	2
1:A:814:LYS:HE2	1:A:821:TRP:CZ2	0.44	2.48	1	1
1:A:790:ARG:NH2	1:A:838:GLU:OE1	0.44	2.50	16	1
1:A:787:ALA:N	1:A:809:ILE:O	0.44	2.50	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:788:LYS:O	1:A:838:GLU:N	0.44	2.50	13	2
1:A:801:LEU:HD11	1:A:824:GLU:CA	0.44	2.43	12	1
1:A:801:LEU:CD1	1:A:823:GLY:C	0.44	2.86	10	2
1:A:796:ARG:CZ	1:A:797:ASP:OD2	0.43	2.65	4	1
1:A:822:ARG:HB2	1:A:831:TRP:CD2	0.43	2.48	10	1
1:A:808:ILE:CG2	1:A:841:TYR:OH	0.43	2.65	13	2
1:A:822:ARG:HD2	1:A:831:TRP:CZ2	0.43	2.48	7	1
1:A:820:TRP:CD1	1:A:831:TRP:CE3	0.43	3.07	4	2
1:A:824:GLU:OE1	1:A:825:ILE:N	0.43	2.50	13	1
1:A:814:LYS:NZ	1:A:839:GLU:CD	0.43	2.72	3	1
1:A:793:PHE:CE2	1:A:833:PRO:CD	0.43	3.01	20	1
1:A:801:LEU:HD13	1:A:830:GLY:N	0.43	2.29	20	1
1:A:790:ARG:NH2	1:A:838:GLU:CD	0.43	2.72	3	2
1:A:787:ALA:CB	1:A:838:GLU:O	0.43	2.67	9	3
1:A:824:GLU:OE2	1:A:825:ILE:N	0.43	2.52	16	2
1:A:839:GLU:O	1:A:841:TYR:N	0.43	2.51	19	8
1:A:789:ALA:HB2	1:A:809:ILE:CD1	0.42	2.44	2	3
1:A:801:LEU:HD22	1:A:832:PHE:CD2	0.42	2.49	20	1
1:A:820:TRP:CZ3	1:A:831:TRP:CD2	0.42	3.07	10	1
1:A:790:ARG:CG	1:A:838:GLU:CD	0.42	2.88	19	1
1:A:814:LYS:HD3	1:A:821:TRP:CE2	0.42	2.49	3	2
1:A:820:TRP:CD2	1:A:831:TRP:CE3	0.42	3.07	10	1
1:A:811:ILE:HG21	1:A:814:LYS:CE	0.42	2.42	7	1
1:A:814:LYS:HD2	1:A:821:TRP:CE2	0.42	2.50	7	3
1:A:833:PRO:HG2	1:A:836:TYR:CD1	0.42	2.50	14	1
1:A:814:LYS:HZ1	1:A:839:GLU:CD	0.42	2.18	3	1
1:A:812:LEU:HD12	1:A:823:GLY:HA2	0.42	1.91	17	1
1:A:801:LEU:CD2	1:A:832:PHE:CD2	0.42	3.02	20	1
1:A:803:LEU:HD11	1:A:809:ILE:CD1	0.41	2.45	14	2
1:A:836:TYR:C	1:A:837:VAL:HG13	0.41	2.35	14	3
1:A:790:ARG:HB2	1:A:791:TYR:CE2	0.41	2.50	13	1
1:A:822:ARG:HG3	1:A:831:TRP:CE2	0.41	2.51	20	2
1:A:821:TRP:CZ3	1:A:839:GLU:OE1	0.41	2.74	3	1
1:A:800:GLU:CG	1:A:801:LEU:N	0.41	2.83	6	1
1:A:791:TYR:CD1	1:A:791:TYR:N	0.41	2.88	10	1
1:A:808:ILE:HG21	1:A:841:TYR:OH	0.41	2.16	13	1
1:A:836:TYR:CD1	1:A:836:TYR:N	0.41	2.89	14	1
1:A:812:LEU:HD12	1:A:823:GLY:CA	0.41	2.46	20	2
1:A:835:ASN:OD1	1:A:835:ASN:N	0.41	2.53	20	1
1:A:821:TRP:CZ3	1:A:834:SER:CB	0.41	3.03	15	1
1:A:792:ASP:OD2	1:A:792:ASP:N	0.40	2.55	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:839:GLU:O	1:A:840:ASP:C	0.40	2.60	5	5
1:A:804:LYS:O	1:A:805:GLU:C	0.40	2.60	11	5
1:A:803:LEU:HD21	1:A:832:PHE:HB2	0.40	1.93	2	1
1:A:824:GLU:OE2	1:A:827:GLY:C	0.40	2.60	10	1
1:A:839:GLU:CD	1:A:839:GLU:C	0.40	2.80	10	1
1:A:795:ALA:O	1:A:796:ARG:C	0.40	2.60	20	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	53/142 (37%)	47±2 (89±3%)	5±1 (10±3%)	0±0 (1±1%)	29	74
All	All	1060/2840 (37%)	948 (89%)	106 (10%)	6 (1%)	29	74

All 3 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	841	TYR	2
1	A	819	GLY	2
1	A	785	GLY	2

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	44/116 (38%)	37±2 (85±4%)	7±2 (15±4%)	6	44
All	All	880/2320 (38%)	749 (85%)	131 (15%)	6	44

All 18 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	808	ILE	20
1	A	801	LEU	19
1	A	820	TRP	18
1	A	803	LEU	12
1	A	802	SER	10
1	A	796	ARG	8
1	A	804	LYS	8
1	A	824	GLU	7
1	A	812	LEU	7
1	A	839	GLU	7
1	A	798	ARG	4
1	A	799	SER	2
1	A	813	ASN	2
1	A	797	ASP	2
1	A	835	ASN	2
1	A	828	ARG	1
1	A	800	GLU	1
1	A	814	LYS	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 [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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	862
Number of shifts mapped to atoms	862
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	69	-0.27 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	60	0.15 ± 0.30	None needed (< 0.5 ppm)
$^{13}\text{C}'$	64	-0.12 ± 0.21	None needed (< 0.5 ppm)
^{15}N	65	-0.23 ± 0.61	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 624 atoms were assigned a chemical shift out of a possible 692. 4 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	261/263 (99%)	105/105 (100%)	104/106 (98%)	52/52 (100%)
Sidechain	289/343 (84%)	179/203 (88%)	106/119 (89%)	4/21 (19%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	74/86 (86%)	44/44 (100%)	27/39 (69%)	3/3 (100%)
Overall	624/692 (90%)	328/352 (93%)	237/264 (90%)	59/76 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 792 atoms were assigned a chemical shift out of a possible 876. 5 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	332/339 (98%)	134/135 (99%)	133/138 (96%)	65/66 (98%)
Sidechain	373/434 (86%)	232/258 (90%)	135/152 (89%)	6/24 (25%)
Aromatic	87/103 (84%)	53/53 (100%)	31/47 (66%)	3/3 (100%)
Overall	792/876 (90%)	419/446 (94%)	299/337 (89%)	74/93 (80%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	814	LYS	HE2	0.94	3.87 – 1.97	-10.4
1	A	822	ARG	HB2	-0.77	3.15 – 0.45	-9.5
1	A	814	LYS	HG2	-0.99	2.67 – 0.07	-9.1
1	A	834	SER	HB2	1.60	5.18 – 2.58	-8.8
1	A	834	SER	HB3	1.85	5.25 – 2.45	-7.1
1	A	833	PRO	HG2	-0.04	3.48 – 0.38	-6.4
1	A	822	ARG	HG2	0.16	2.92 – 0.22	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

