



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 PM UTC

PDB ID : 2KBT / pdb_00002kbt
BMRB ID : 16053
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 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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

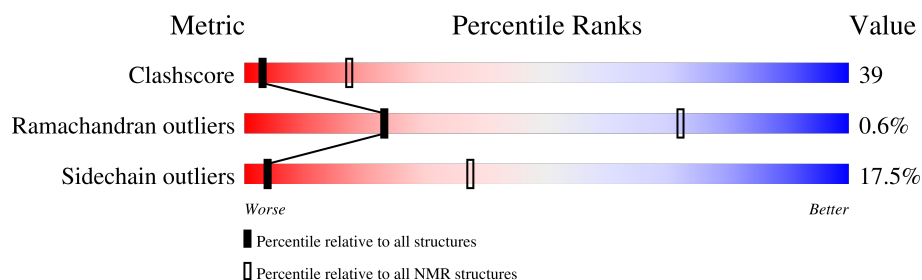
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	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)	0.41	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 Proto-oncogene vav,Immunoglobulin G-binding protein G.

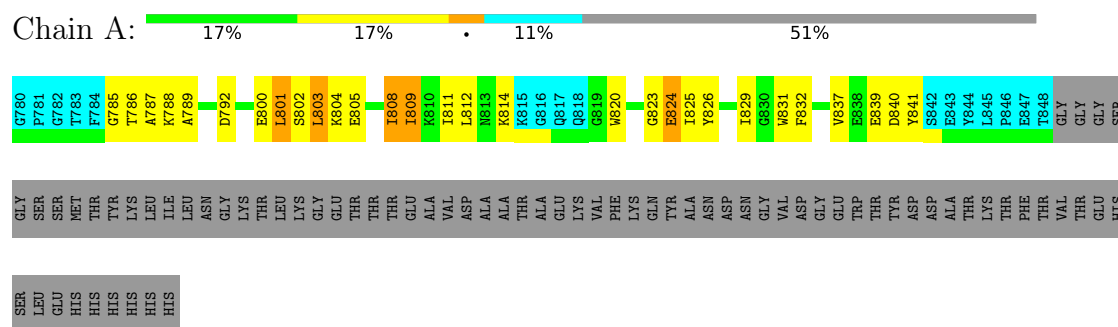
Mol	Chain	Residues	Atoms						Trace
1	A	69	Total	C	H	N	O	S	0
			1102	362	536	96	107	1	

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	-	linker	UNP P27870
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

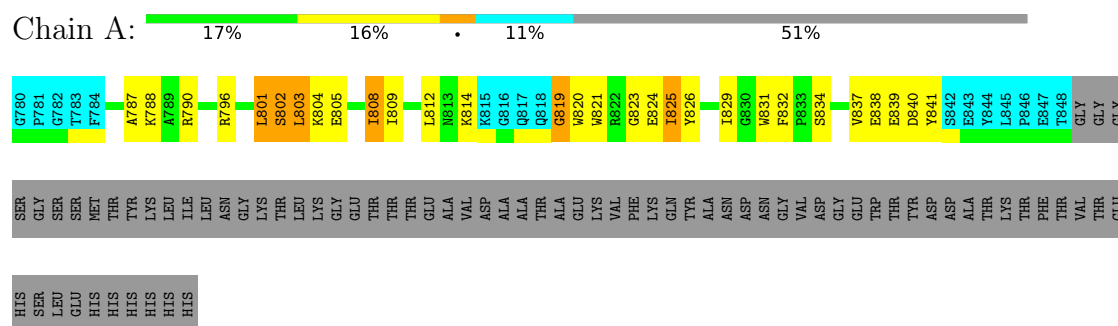
4.2.2 Score per residue for model 2

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



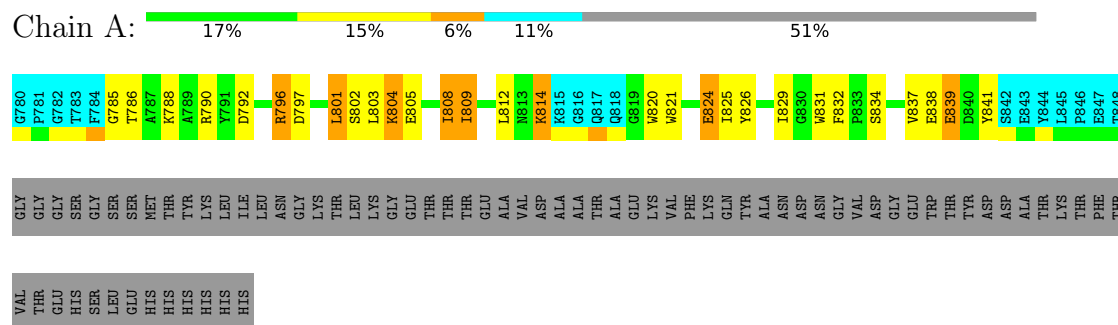
4.2.3 Score per residue for model 3

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



4.2.4 Score per residue for model 4

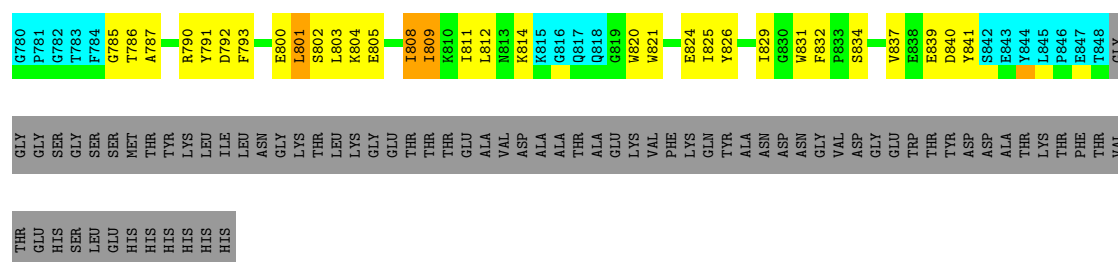
- Molecule 1: Proto-oncogene vav,Immunoglobulin G-binding protein G



4.2.5 Score per residue for model 5

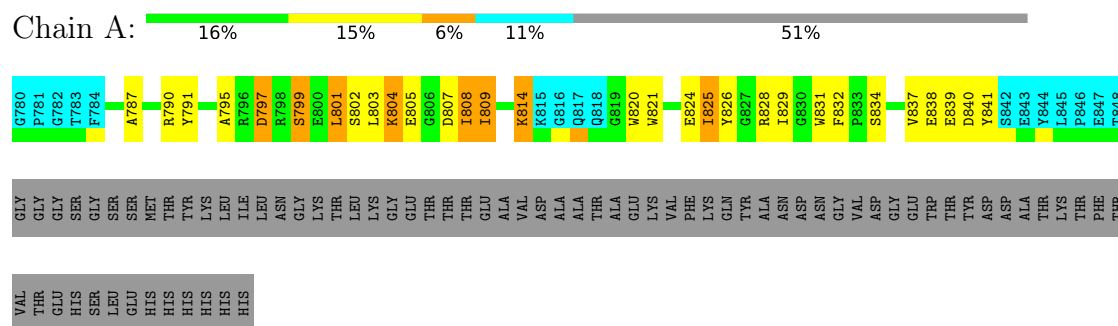
- Molecule 1: Proto-oncogene vav,Immunoglobulin G-binding protein G





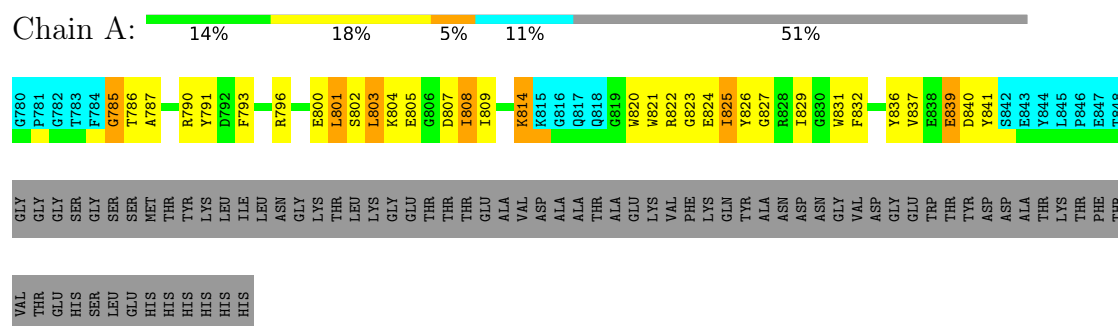
4.2.9 Score per residue for model 9

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



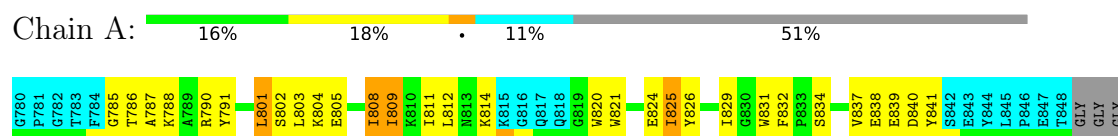
4.2.10 Score per residue for model 10

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



4.2.11 Score per residue for model 11

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



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

HIS SER LEU LEU HIS HIS HIS HIS HIS HIS

4.2.12 Score per residue for model 12

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

Chain A: 15% 18% • 11% 51%

G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G796 L801 L802 L803 L804 L805 L808 L809 L810 L811 L812 L813 L814 L815 L816 L817 L818 L819 L820 L821 L824 L825 L826 L829 L830 L831 L832 L833 L834 L837 L838 L839 L840 L841 L842 L843 L844 L845 L846 L847 L848 GLY

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

THR GLU HIS LEU GLU HIS HIS HIS HIS HIS HIS

4.2.13 Score per residue for model 13

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

Chain A: 18% 18% • 11% 51%

G780 G781 G782 G783 G784 G788 G789 G790 G791 G796 L801 L802 L803 L804 L805 L808 L809 L812 L813 L814 L815 L816 L817 L818 L819 L820 L821 L822 L823 L824 L825 L826 L829 L830 L831 L832 L833 L837 L838 L839 L840 L841 L842 L843 L844 L845 L846 L847 L848 GLY GLY GLY GLY

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

LEU GLU HIS HIS HIS HIS HIS HIS

4.2.14 Score per residue for model 14

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

Chain A: 15% 16% 6% 11% 51%

G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G796 L801 L802 L803 L804 L805 L806 L807 L808 L809 L812 L813 L814 L815 L816 L817 L818 L819 L820 L821 L822 L823 L824 L825 L826 L829 L830 L831 L832 L833 L834 L835 L836 L837 L838 L839 L840 L841 L842 L843 L844 L845 L846 L847 L848 GLY

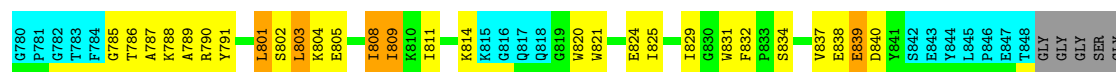
GLY SER GLY SER SER MET THR TYR LYS LEU LEU ILE LEU ASN GLY LYS THR THR THR THR VAL ASP THR ALA THR THR THR LYS GLU VAL PHE LYS GLN TYR ALA ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ASP THR ALA LYS THR PHE THR LYS THR VAL THR THR GLY

GLU
HIS
SER
LEU
GLU
HIS
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HIS
HIS

4.2.15 Score per residue for model 15 (medoid)

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

Chain A: 18% 16% • 11% 51%



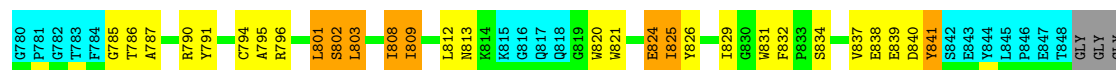
SER
SER
MET
THR
TYR
LYS
LEU
ILE
LEU
ASN
GLY
LYS
THR
LEU
LEU
GLY
VAL
ASP
ALA
ALA
THR
GLU
GLU
LYS
VAL
PHE
LYS
GLN
TYR
ALA
ASN
ASP
ASN
GLY
VAL
ASP
GLY
GLU
TRP
THR
TYR
ASP
ASP
ALA
THR
LYS
THR
PHE
THR
VAL
THR
GLY
GLY
SER
GLY

LEU
GLU
HIS
HIS
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HIS
HIS
HIS

4.2.16 Score per residue for model 16

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

Chain A: 17% 15% 6% 11% 51%



SER
GLY
SER
SER
SER
MET
THR
TYR
LYS
LEU
ILE
LEU
ASN
GLY
LYS
THR
LYS
GLY
GLY
GLU
THR
THR
THR
THR
GLU
VAL
ASP
ALA
ALA
THR
GLU
GLU
LYS
VAL
PHE
LYS
GLN
TYR
ALA
ASN
ASP
ASN
GLY
VAL
ASP
GLY
GLU
TRP
THR
TYR
D840
ASP
ASP
ALA
THR
LYS
THR
PHE
THR
VAL
THR
GLY
GLY

HIS
SER
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4.2.17 Score per residue for model 17

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

Chain A: 19% 13% 5% 11% 51%

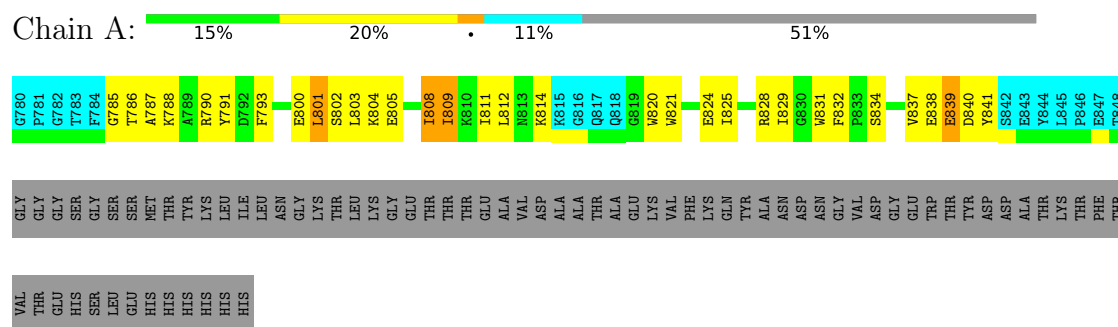


SER
SER
MET
THR
TYR
LYS
LEU
ILE
LEU
ASN
GLY
LYS
THR
LEU
LEU
GLY
GLU
THR
THR
THR
GLU
VAL
ASP
ASP
ALA
ALA
THR
GLU
GLU
LYS
VAL
PHE
LYS
GLN
TYR
ALA
ASN
ASP
ASN
GLY
VAL
ASP
GLY
GLU
TRP
THR
TYR
ASP
ASP
ALA
THR
LYS
THR
PHE
THR
VAL
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GLY
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SER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

LEU
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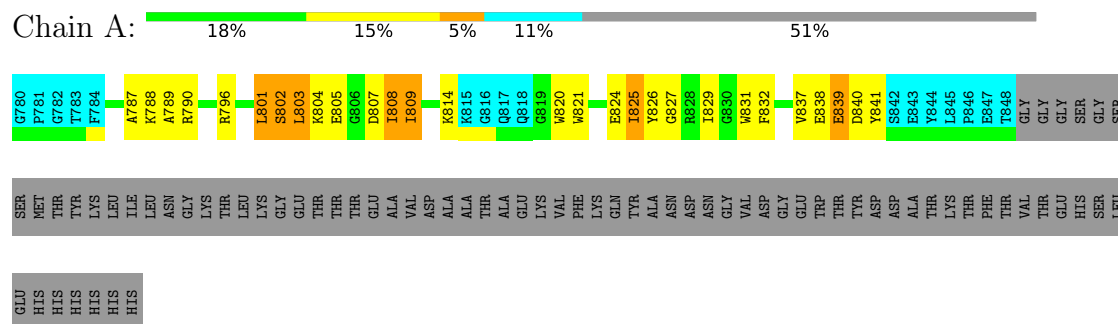
4.2.18 Score per residue for model 18

- Molecule 1: Proto-oncogene *vav*, Immunoglobulin G-binding protein G



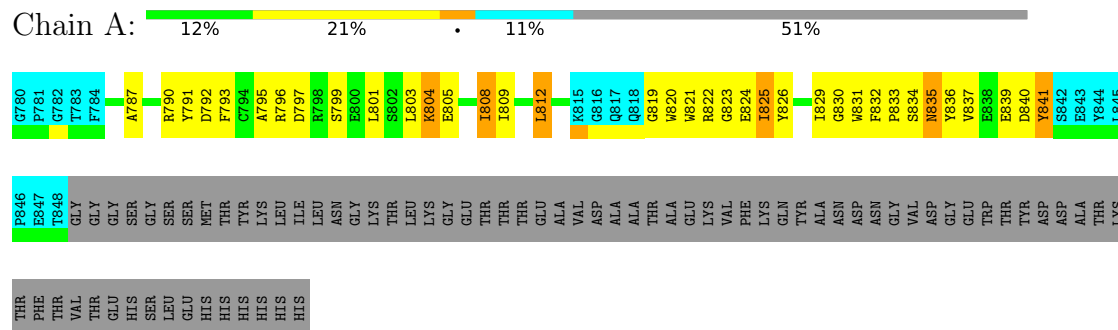
4.2.19 Score per residue for model 19

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



4.2.20 Score per residue for model 20

- Molecule 1: Proto-oncogene vav, 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)	working_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)	91%

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	34±7
All	All	8880	8460	8460	676

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 39.

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:HD13	1:A:808:ILE:N	0.71	2.01	10	20
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:790:ARG:C	1:A:791:TYR:CD1	0.64	2.75	14	9
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:793:PHE:CE2	1:A:800:GLU:CD	0.60	2.79	6	4
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: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:801:LEU:HD11	1:A:823:GLY:C	0.57	2.24	10	4
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:OE1	0.55	2.59	10	1
1:A:790:ARG:C	1:A:791:TYR:CG	0.54	2.86	18	10
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:796:ARG:CZ	1:A:797:ASP:CG	0.53	2.81	4	1
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	10
1:A:808:ILE:N	1:A:808:ILE:CD1	0.52	2.70	16	15
1:A:811:ILE:HG21	1:A:814:LYS:HZ3	0.52	1.63	7	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:814:LYS:HZ1	1:A:839:GLU:CD	0.50	2.15	3	1
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:839:GLU:CD	1:A:839:GLU:C	0.50	2.80	10	3
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:790:ARG:C	1:A:791:TYR:CD2	0.50	2.90	8	3
1:A:808:ILE:O	1:A:825:ILE:CD1	0.49	2.60	7	7
1:A:820:TRP:CE3	1:A:831:TRP:HB3	0.49	2.42	11	14
1:A:839:GLU:C	1:A:841:TYR:N	0.49	2.70	8	12
1:A:793:PHE:CZ	1:A:833:PRO:HG3	0.49	2.42	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:785:GLY:O	1:A:786:THR:CG2	0.49	2.60	10	4
1:A:814:LYS:CE	1:A:821:TRP:CE2	0.49	2.96	1	1
1:A:812:LEU:HB3	1:A:822:ARG:HH21	0.49	1.66	14	1
1:A:801:LEU:CD1	1:A:823:GLY:C	0.48	2.86	10	3
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:824:GLU:CD	1:A:824:GLU:C	0.48	2.81	13	4
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:821:TRP:CZ3	1:A:834:SER:OG	0.48	2.59	12	1
1:A:814:LYS:NZ	1:A:821:TRP:CE3	0.48	2.81	3	1
1:A:814:LYS:NZ	1:A:839:GLU:CD	0.48	2.72	3	1
1:A:790:ARG:NH2	1:A:838:GLU:CD	0.47	2.72	3	2
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:838:GLU:C	1:A:839:GLU:CD	0.47	2.82	16	2
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:790:ARG:CG	1:A:838:GLU:CD	0.47	2.88	19	1
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:836:TYR:C	1:A:837:VAL:HG13	0.46	2.35	14	4
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:826:TYR:CD1	1:A:826:TYR:N	0.45	2.80	8	3
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:839:GLU:O	1:A:840:ASP:C	0.45	2.60	5	15
1:A:804:LYS:O	1:A:805:GLU:C	0.45	2.60	2	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:824:GLU:OE2	1:A:827:GLY:C	0.45	2.60	10	4
1:A:795:ALA:O	1:A:796:ARG:C	0.45	2.60	20	1
1:A:790:ARG:O	1:A:790:ARG:NH1	0.45	2.50	7	1
1:A:804:LYS:O	1:A:807:ASP:CG	0.45	2.60	10	5
1:A:824:GLU:OE2	1:A:825:ILE:CA	0.45	2.65	16	2
1:A:840:ASP:CG	1:A:840:ASP:O	0.44	2.60	10	8
1:A:813:ASN:OD1	1:A:813:ASN:C	0.44	2.59	13	1
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
1:A:821:TRP:CZ3	1:A:839:GLU:CD	0.44	2.96	12	1
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: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:836:TYR:C	1:A:837:VAL:CG1	0.43	2.92	20	3
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:790:ARG:C	1:A:805:GLU:CG	0.43	2.91	4	2
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: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: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:814:LYS:HD3	1:A:821:TRP:CE2	0.42	2.49	3	2
1:A:797:ASP:CG	1:A:799:SER:OG	0.42	2.62	9	1
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:795:ALA:C	1:A:797:ASP:N	0.42	2.76	9	2
1:A:812:LEU:HD12	1:A:823:GLY:HA2	0.42	1.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:797:ASP:CG	1:A:799:SER:HG	0.42	2.22	9	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:790:ARG:HB2	1:A:791:TYR:CE2	0.41	2.50	13	1
1:A:807:ASP:CG	1:A:826:TYR:OH	0.41	2.63	14	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:785:GLY:C	1:A:786:THR:HG23	0.41	2.41	16	2
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:794:CYS:O	1:A:795:ALA:C	0.41	2.64	16	1
1:A:824:GLU:OE2	1:A:824:GLU:C	0.40	2.64	16	1
1:A:839:GLU:C	1:A:839:GLU:CD	0.40	2.89	17	1
1:A:792:ASP:OD2	1:A:792:ASP:N	0.40	2.55	20	1
1:A:803:LEU:HD21	1:A:832:PHE:HB2	0.40	1.93	2	1
1:A:800:GLU:CD	1:A:831:TRP:O	0.40	2.64	2	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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%)	23	72
All	All	1060/2840 (37%)	948 (89%)	106 (10%)	6 (1%)	23	72

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	819	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	785	GLY	2
1	A	841	TYR	2

6.3.2 Protein sidechains ⓘ

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%)	36±2 (82±4%)	8±2 (18±4%)	4	37
All	All	880/2320 (38%)	726 (82%)	154 (18%)	4	37

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	803	LEU	20
1	A	808	ILE	20
1	A	801	LEU	19
1	A	812	LEU	16
1	A	825	ILE	15
1	A	809	ILE	14
1	A	824	GLU	7
1	A	839	GLU	7
1	A	796	ARG	7
1	A	802	SER	6
1	A	814	LYS	6
1	A	804	LYS	6
1	A	792	ASP	3
1	A	797	ASP	2
1	A	799	SER	2
1	A	813	ASN	2
1	A	798	ARG	1
1	A	835	ASN	1

6.3.3 RNA ⓘ

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 oligosaccharides 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_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)	8

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 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	60	0.16 ± 0.31	None needed (< 0.5 ppm)
$^{13}\text{C}'$	64	-0.12 ± 0.15	None needed (< 0.5 ppm)
^{15}N	65	-0.23 ± 0.33	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 91%, i.e. 678 atoms were assigned a chemical shift out of a possible 748. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	267/269 (99%)	111/111 (100%)	104/106 (98%)	52/52 (100%)
Sidechain	335/387 (87%)	224/247 (91%)	107/119 (90%)	4/21 (19%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	76/92 (83%)	44/44 (100%)	29/45 (64%)	3/3 (100%)
Overall	678/748 (91%)	379/402 (94%)	240/270 (89%)	59/76 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 862 atoms were assigned a chemical shift out of a possible 945. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	341/348 (98%)	143/144 (99%)	133/138 (96%)	65/66 (98%)
Sidechain	431/486 (89%)	287/310 (93%)	138/152 (91%)	6/24 (25%)
Aromatic	90/111 (81%)	53/53 (100%)	34/55 (62%)	3/3 (100%)
Overall	862/945 (91%)	483/507 (95%)	305/345 (88%)	74/93 (80%)

7.1.4 Statistically unusual chemical shifts ⓘ

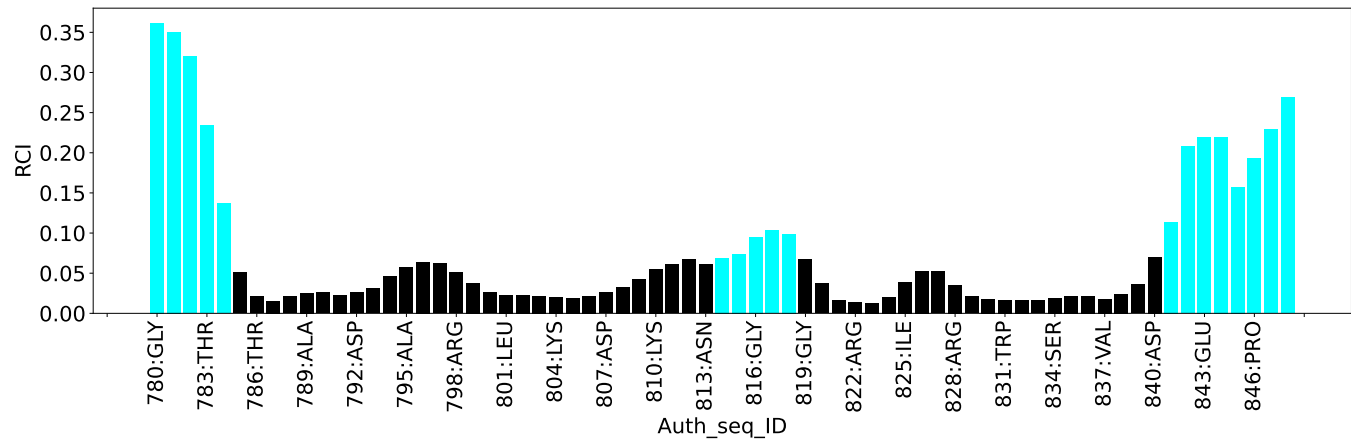
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	814	LYS	HE2	0.94	1.95 – 3.88	-10.2
1	A	822	ARG	HB2	-0.77	0.52 – 3.08	-10.0
1	A	814	LYS	HG2	-0.99	0.13 – 2.61	-9.5
1	A	834	SER	HB2	1.60	2.61 – 5.13	-9.0
1	A	834	SER	HB3	1.85	2.49 – 5.20	-7.4
1	A	833	PRO	HG2	-0.04	0.41 – 3.45	-6.5
1	A	822	ARG	HG2	0.16	0.26 – 2.87	-5.4
1	A	814	LYS	CD	34.56	23.50 – 34.42	5.1

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1051
Intra-residue ($ i-j =0$)	281
Sequential ($ i-j =1$)	309
Medium range ($ i-j >1$ and $ i-j <5$)	75
Long range ($ i-j \geq 5$)	386
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	7.4
Number of long range restraints per residue ¹	2.7

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.6	0.2
0.2-0.5 (Medium)	0.5	0.47
>0.5 (Large)	1.9	1.6

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

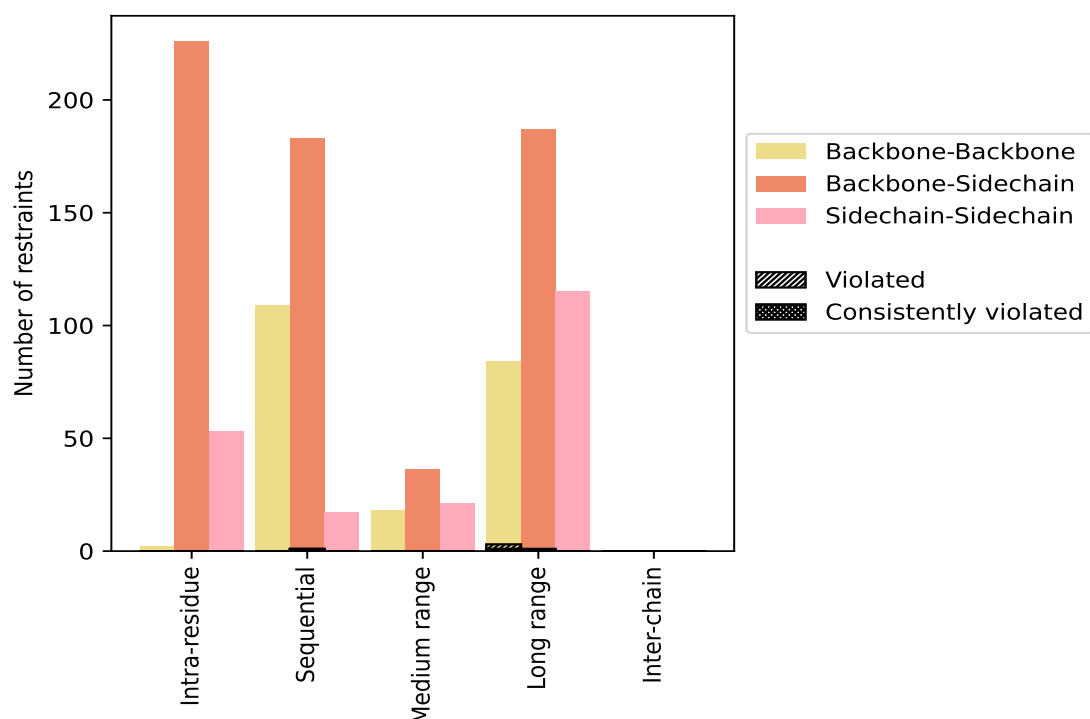
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	281	26.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	226	21.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	53	5.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	309	29.4	1	0.3	0.1	1	0.3	0.1
Backbone-Backbone	109	10.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	183	17.4	1	0.5	0.1	1	0.5	0.1
Sidechain-Sidechain	17	1.6	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	75	7.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	18	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	36	3.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	21	2.0	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	386	36.7	4	1.0	0.4	1	0.3	0.1
Backbone-Backbone	84	8.0	3	3.6	0.3	1	1.2	0.1
Backbone-Sidechain	187	17.8	1	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	115	10.9	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1051	100.0	5	0.5	0.5	2	0.2	0.2
Backbone-Backbone	213	20.3	3	1.4	0.3	1	0.5	0.1
Backbone-Sidechain	632	60.1	2	0.3	0.2	1	0.2	0.1
Sidechain-Sidechain	206	19.6	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	1	0	2	0	3	0.81	1.24	0.39	0.89
2	0	1	0	1	0	2	1.0	1.24	0.24	1.0
3	0	1	0	2	0	3	0.93	1.6	0.53	0.89
4	0	1	0	2	0	3	0.64	1.0	0.34	0.75
5	0	1	0	1	0	2	1.0	1.27	0.27	1.0
6	0	1	0	2	0	3	0.76	1.28	0.44	0.81
7	0	1	0	1	0	2	1.05	1.48	0.43	1.05
8	0	1	0	3	0	4	0.61	1.23	0.41	0.51
9	0	1	0	2	0	3	0.74	1.28	0.46	0.78
10	0	1	0	2	0	3	0.63	0.99	0.37	0.78

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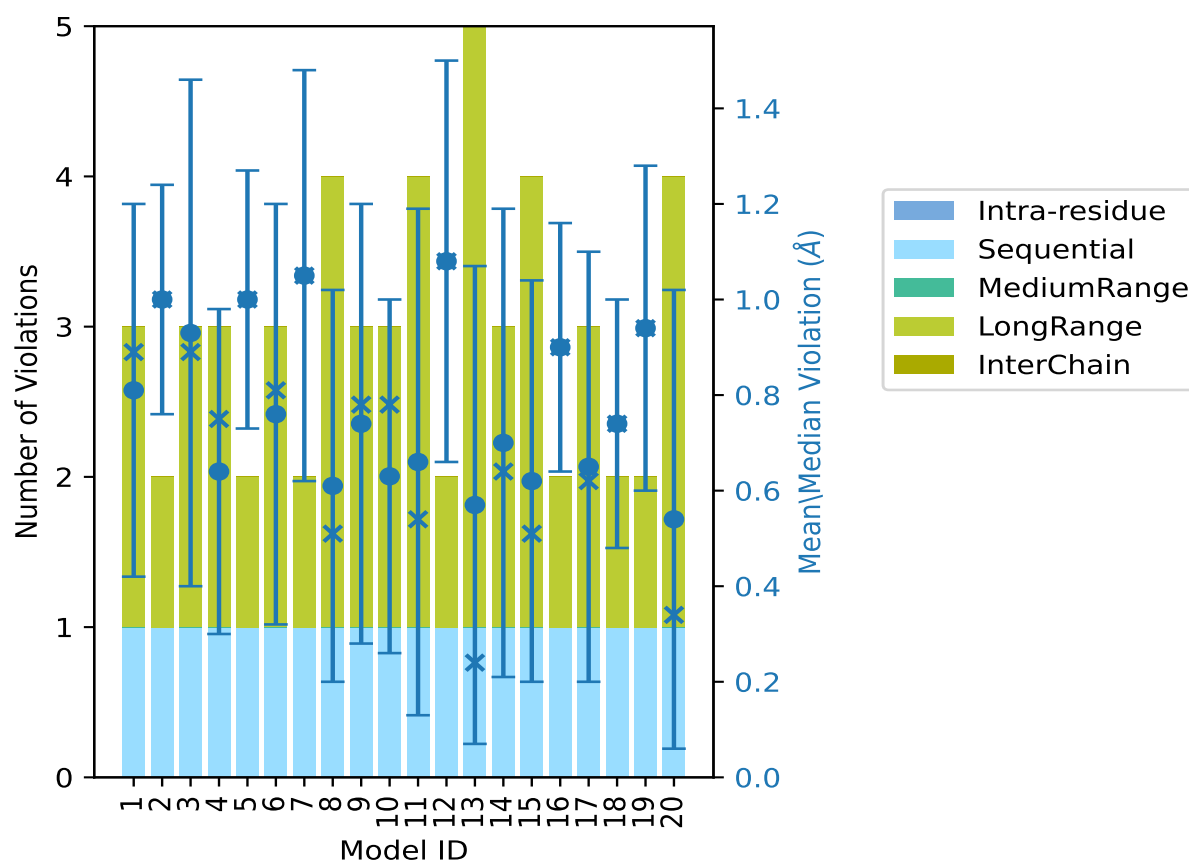
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	0	3	0	4	0.66	1.45	0.53	0.54
12	0	1	0	1	0	2	1.08	1.49	0.42	1.08
13	0	1	0	4	0	5	0.57	1.5	0.5	0.24
14	0	1	0	2	0	3	0.7	1.33	0.49	0.64
15	0	1	0	3	0	4	0.62	1.23	0.42	0.51
16	0	1	0	1	0	2	0.9	1.17	0.26	0.9
17	0	1	0	2	0	3	0.65	1.22	0.45	0.62
18	0	1	0	1	0	2	0.74	1.0	0.26	0.74
19	0	1	0	1	0	2	0.94	1.28	0.34	0.94
20	0	1	0	3	0	4	0.54	1.31	0.48	0.34

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

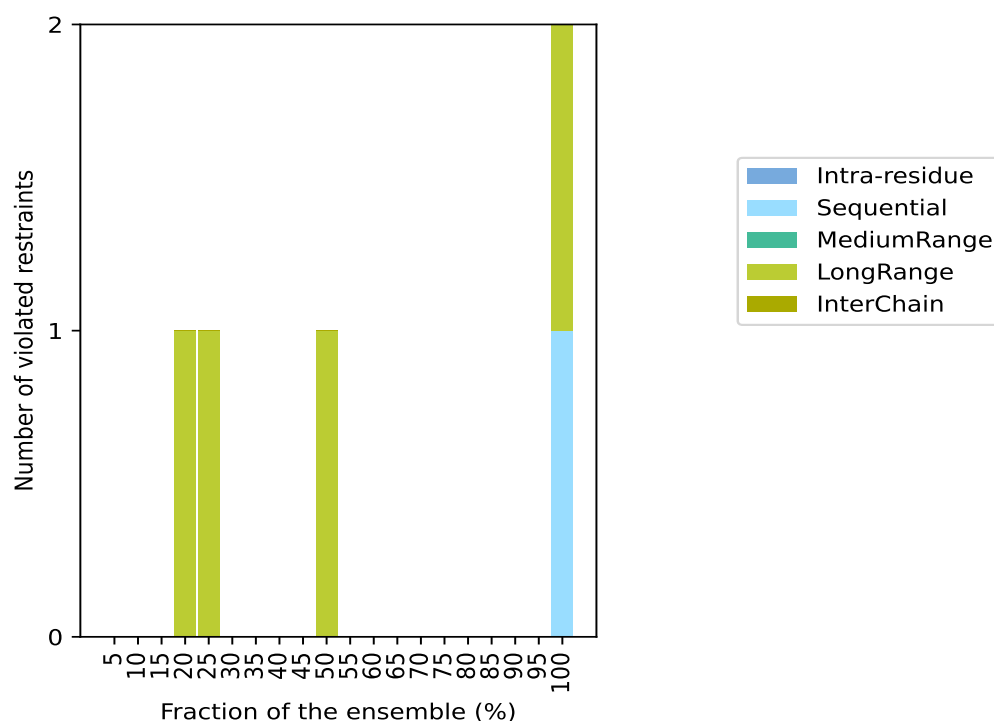
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1046(IR:281, SQ:308, MR:75, LR:382, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	1	0	1	4	20.0
0	0	0	1	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	1	0	1	0	2	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

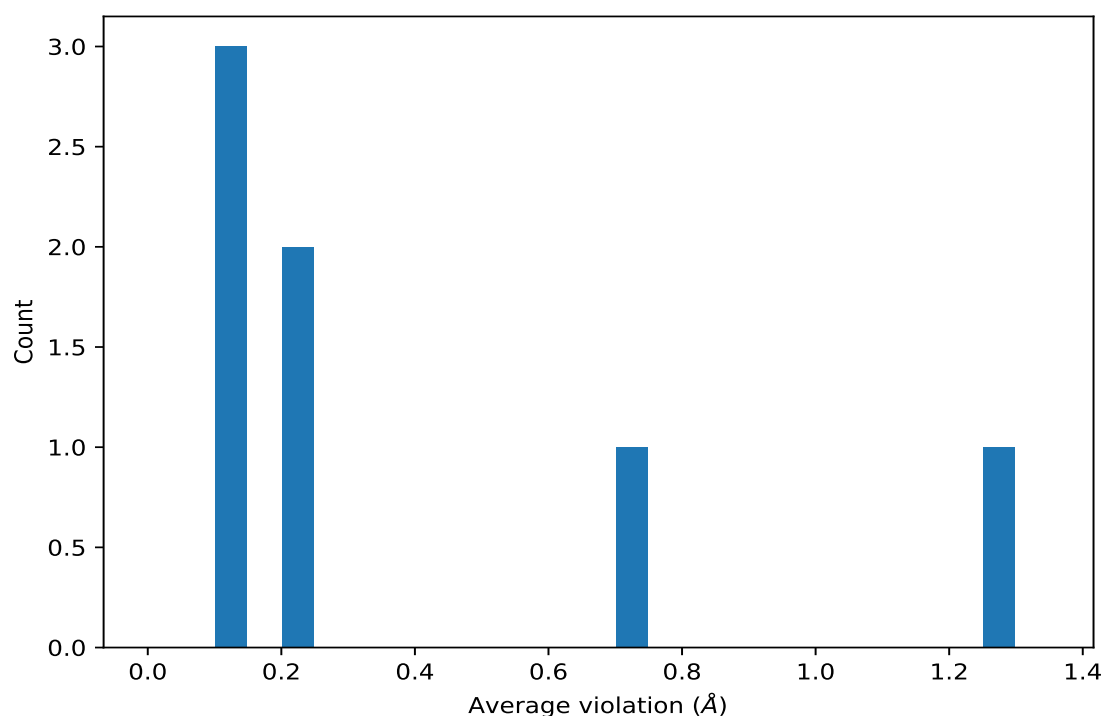
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

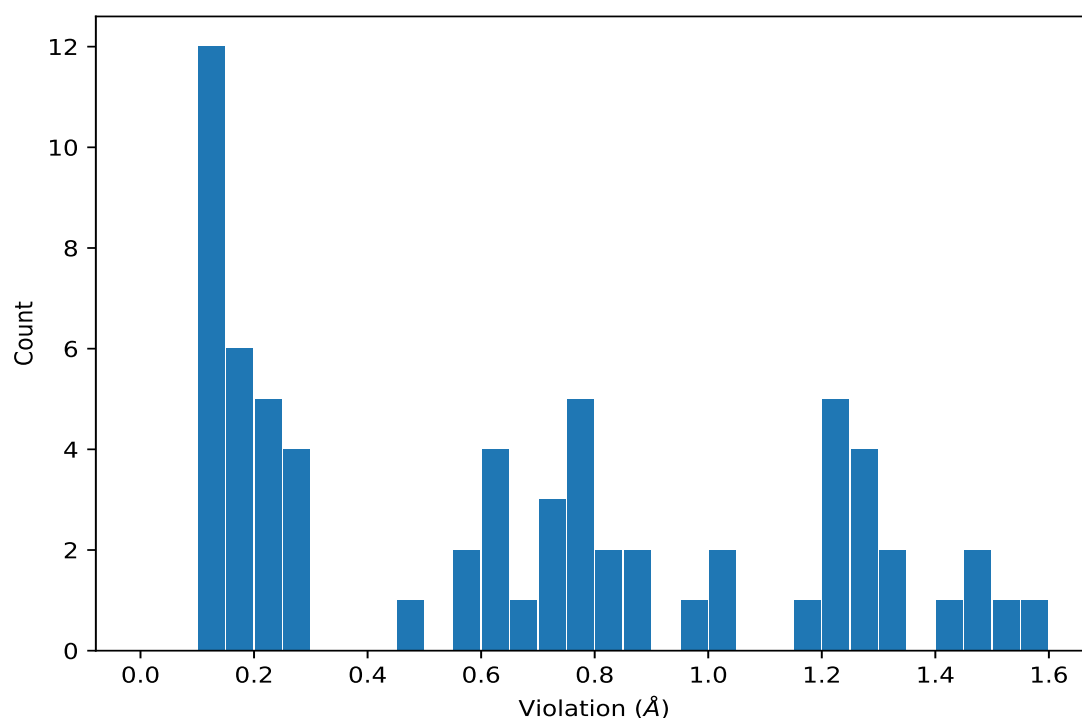
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	20	1.28	0.16	1.27
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	20	0.71	0.11	0.72
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	10	0.21	0.05	0.21
(1,392)	1:810:A:LYS:H	1:823:A:GLY:HA2	5	0.21	0.07	0.24
(1,553)	1:809:A:ILE:HG21	1:823:A:GLY:HA2	4	0.14	0.02	0.14
(1,553)	1:809:A:ILE:HG22	1:823:A:GLY:HA2	4	0.14	0.02	0.14
(1,553)	1:809:A:ILE:HG23	1:823:A:GLY:HA2	4	0.14	0.02	0.14

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	3	1.6
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	13	1.5
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	12	1.49
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	7	1.48
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	11	1.45
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	14	1.33
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	20	1.31
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	6	1.28
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	9	1.28
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	19	1.28
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	5	1.27
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	1	1.24
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	2	1.24
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	8	1.23
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	15	1.23
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	17	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	16	1.17
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	4	1.0
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	18	1.0
(1,470)	1:819:A:GLY:HA2	1:820:A:TRP:HE1	10	0.99
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	1	0.89
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	3	0.89
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	11	0.84
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	6	0.81
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	9	0.78
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	10	0.78
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	15	0.77
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	2	0.76
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	4	0.75
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	5	0.73
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	8	0.72
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	13	0.72
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	12	0.66
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	14	0.64
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	16	0.64
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	7	0.62
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	17	0.62
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	19	0.6
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	20	0.55
(1,43)	1:813:A:ASN:H	1:823:A:GLY:HA3	18	0.47
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	3	0.3
(1,392)	1:810:A:LYS:H	1:823:A:GLY:HA2	8	0.3
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	1	0.29
(1,392)	1:810:A:LYS:H	1:823:A:GLY:HA2	15	0.25
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	13	0.24
(1,392)	1:810:A:LYS:H	1:823:A:GLY:HA2	13	0.24
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	11	0.23
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	15	0.22
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	6	0.2
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	4	0.18
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	8	0.18
(1,553)	1:809:A:ILE:HG21	1:823:A:GLY:HA2	13	0.17
(1,553)	1:809:A:ILE:HG22	1:823:A:GLY:HA2	13	0.17
(1,553)	1:809:A:ILE:HG23	1:823:A:GLY:HA2	13	0.17
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	9	0.16
(1,553)	1:809:A:ILE:HG21	1:823:A:GLY:HA2	14	0.14
(1,553)	1:809:A:ILE:HG22	1:823:A:GLY:HA2	14	0.14
(1,553)	1:809:A:ILE:HG23	1:823:A:GLY:HA2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:809:A:ILE:HG21	1:823:A:GLY:HA2	20	0.14
(1,553)	1:809:A:ILE:HG22	1:823:A:GLY:HA2	20	0.14
(1,553)	1:809:A:ILE:HG23	1:823:A:GLY:HA2	20	0.14
(1,392)	1:810:A:LYS:H	1:823:A:GLY:HA2	20	0.14
(1,433)	1:812:A:LEU:H	1:823:A:GLY:HA3	10	0.13
(1,392)	1:810:A:LYS:H	1:823:A:GLY:HA2	11	0.12
(1,553)	1:809:A:ILE:HG21	1:823:A:GLY:HA2	17	0.11
(1,553)	1:809:A:ILE:HG22	1:823:A:GLY:HA2	17	0.11
(1,553)	1:809:A:ILE:HG23	1:823:A:GLY:HA2	17	0.11

10 Dihedral-angle violation analysis

No dihedral-angle restraints found