



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:49 PM UTC

PDB ID : 6WA3 / pdb_00006wa3
BMRB ID : 30738
Title : Solution NMR structure of the myristoylated feline immunodeficiency virus matrix protein
Authors : Brown, J.B.; Summers, H.R.; Brown, L.A.; Marchant, J.; Canova, P.N.; O'Hern, C.T.; Abbott, S.; Nyaunu, C.; Maxwell, S.; Johnson, T.; Moser, M.; Ablan, S.D.; Carter, H.; Freed, E.O.; Summers, M.F.
Deposited on : 2020-03-24

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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

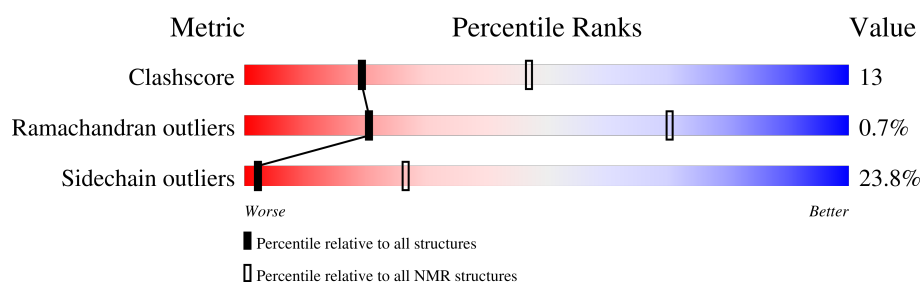
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	124	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:8-A:21, A:28-A:113 (100)	0.58	1

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1850 atoms, of which 938 are hydrogens and 0 are deuteriums.

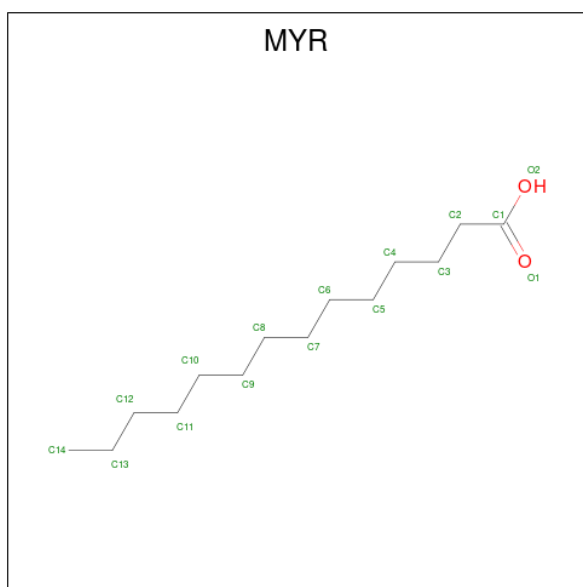
- Molecule 1 is a protein called Matrix protein.

Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1808	556	911	165	168	8	

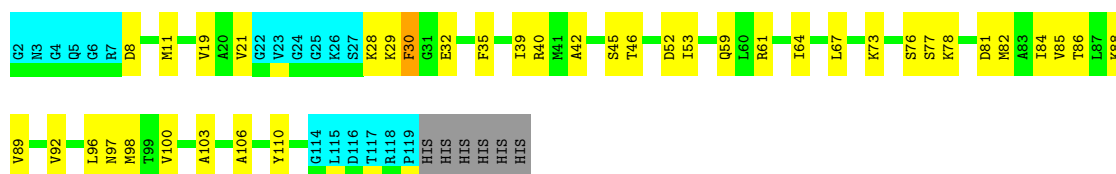
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	HIS	-	expression tag	UNP Q66971
A	121	HIS	-	expression tag	UNP Q66971
A	122	HIS	-	expression tag	UNP Q66971
A	123	HIS	-	expression tag	UNP Q66971
A	124	HIS	-	expression tag	UNP Q66971
A	125	HIS	-	expression tag	UNP Q66971

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).

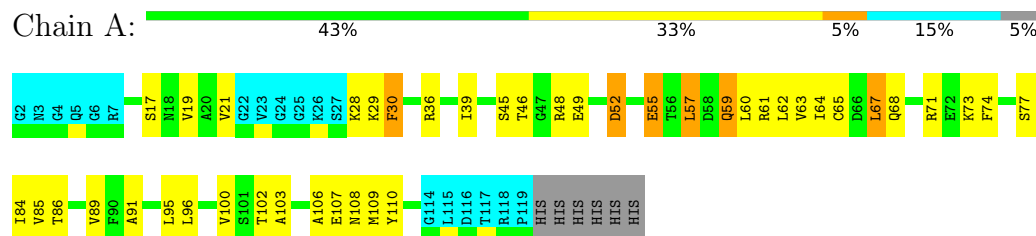


Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			42	14	27	1



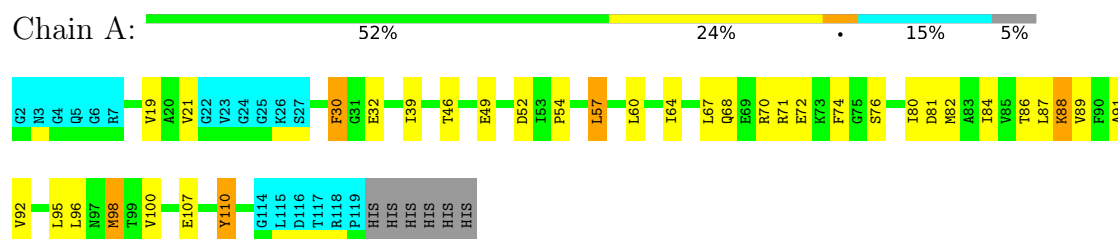
4.2.3 Score per residue for model 3

- Molecule 1: Matrix protein



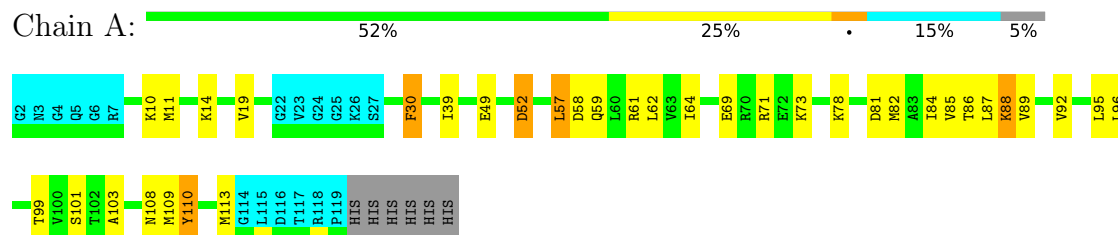
4.2.4 Score per residue for model 4

- Molecule 1: Matrix protein



4.2.5 Score per residue for model 5

- Molecule 1: Matrix protein

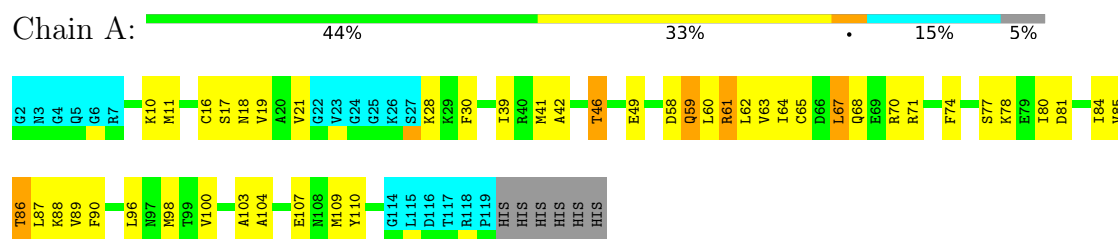


4.2.6 Score per residue for model 6

- Molecule 1: Matrix protein

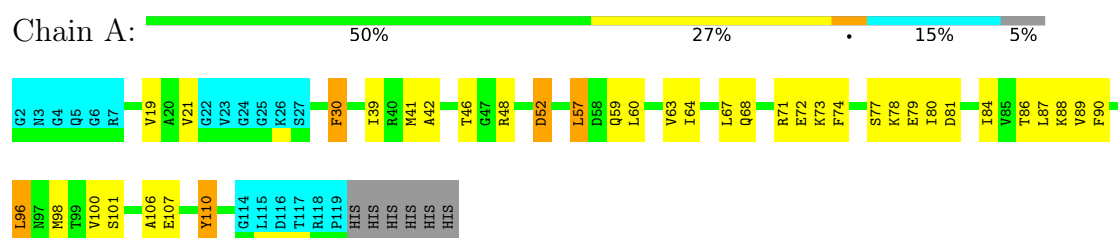
4.2.14 Score per residue for model 14

- Molecule 1: Matrix protein



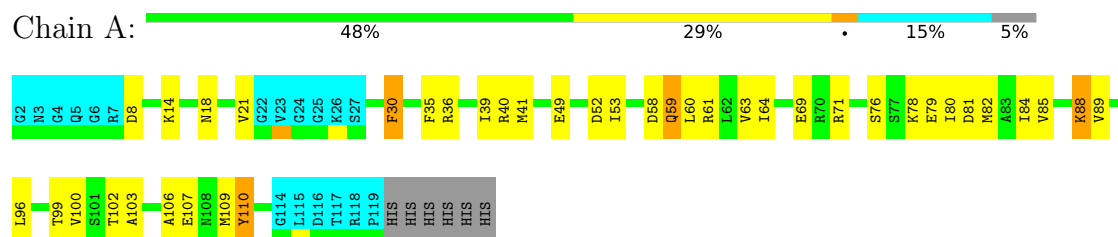
4.2.15 Score per residue for model 15

- Molecule 1: Matrix protein



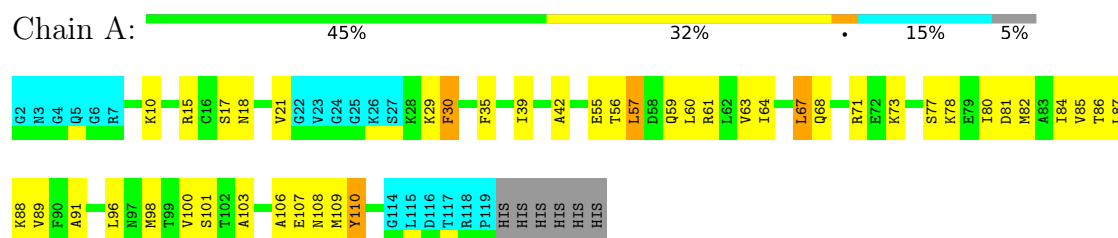
4.2.16 Score per residue for model 16

- Molecule 1: Matrix protein



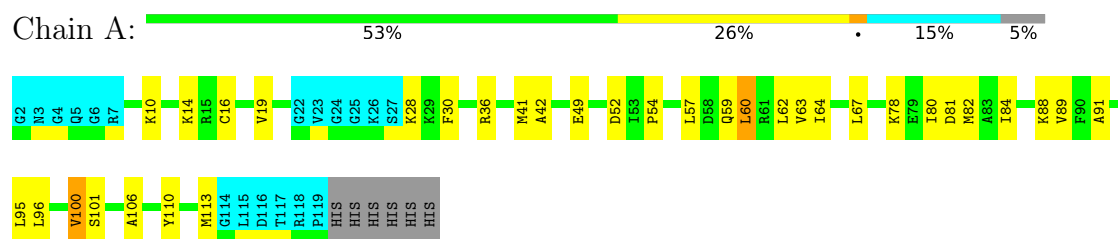
4.2.17 Score per residue for model 17

- Molecule 1: Matrix protein



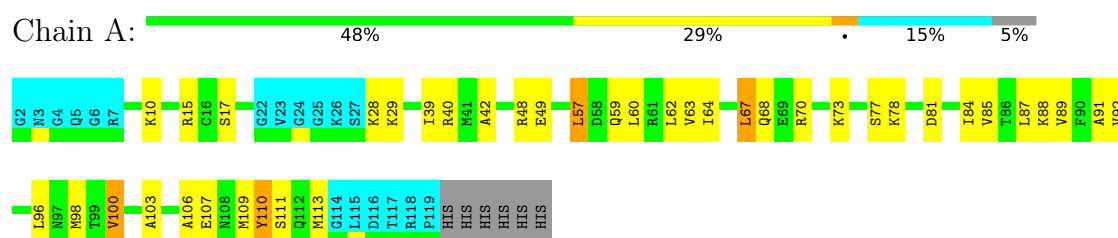
4.2.18 Score per residue for model 18

- Molecule 1: Matrix protein



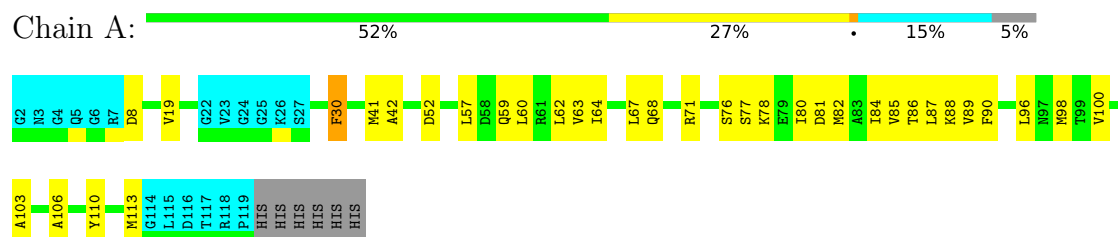
4.2.19 Score per residue for model 19

- Molecule 1: Matrix protein



4.2.20 Score per residue for model 20

- Molecule 1: Matrix protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 200 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
CYANA	refinement	
CYANA	structure calculation	

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	1166
Number of shifts mapped to atoms	1166
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MYR

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	778	794	794	20±4
2	A	15	27	27	2±2
All	All	15860	16420	16420	406

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ILE:HG23	1:A:84:ILE:HG23	0.89	1.45	3	18
1:A:39:ILE:HG22	1:A:87:LEU:HD21	0.83	1.50	7	3
1:A:100:VAL:HG21	1:A:106:ALA:HB2	0.81	1.51	7	4
1:A:87:LEU:HD23	2:A:201:MYR:H141	0.81	1.52	17	2
1:A:67:LEU:HD12	1:A:80:ILE:HG23	0.79	1.53	3	2
1:A:89:VAL:HG23	1:A:100:VAL:HG21	0.78	1.56	19	3
1:A:39:ILE:HD12	2:A:201:MYR:H143	0.77	1.57	11	5
1:A:19:VAL:HG11	1:A:89:VAL:HG21	0.76	1.57	4	9
1:A:60:LEU:HD21	2:A:201:MYR:H141	0.76	1.56	20	1
1:A:89:VAL:HG22	1:A:106:ALA:HB3	0.75	1.58	10	6
1:A:60:LEU:HD11	2:A:201:MYR:H141	0.73	1.58	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:HG12	1:A:103:ALA:HB1	0.72	1.61	7	7
1:A:80:ILE:HG22	1:A:84:ILE:HD11	0.71	1.61	9	5
1:A:19:VAL:HG21	1:A:89:VAL:HG21	0.70	1.62	18	2
1:A:85:VAL:HG11	1:A:103:ALA:HB1	0.69	1.64	17	5
1:A:42:ALA:HB1	1:A:67:LEU:HD11	0.68	1.65	20	3
1:A:16:CYS:O	1:A:19:VAL:HG22	0.66	1.91	18	2
1:A:60:LEU:HD23	1:A:87:LEU:HD22	0.65	1.68	19	1
1:A:35:PHE:CZ	1:A:39:ILE:HD11	0.65	2.27	16	3
1:A:39:ILE:HD12	2:A:201:MYR:H141	0.64	1.68	5	2
1:A:21:VAL:HG22	1:A:30:PHE:CD1	0.64	2.28	15	5
1:A:64:ILE:HG21	1:A:88:LYS:HE2	0.64	1.70	18	1
1:A:59:GLN:O	1:A:63:VAL:HG23	0.63	1.94	14	15
1:A:92:VAL:HG22	1:A:110:TYR:CE2	0.63	2.28	5	1
1:A:46:THR:HG23	1:A:67:LEU:HD22	0.63	1.69	3	2
1:A:92:VAL:HG22	1:A:98:MET:HB2	0.63	1.69	9	4
1:A:16:CYS:O	1:A:19:VAL:HG12	0.63	1.94	14	1
1:A:87:LEU:CD2	2:A:201:MYR:H141	0.63	2.24	17	2
1:A:100:VAL:HG11	1:A:106:ALA:HB2	0.63	1.70	15	10
1:A:71:ARG:HB2	1:A:80:ILE:HG21	0.62	1.70	17	12
1:A:64:ILE:HG21	1:A:88:LYS:CE	0.62	2.23	18	2
1:A:30:PHE:CZ	1:A:86:THR:HG23	0.62	2.29	17	12
1:A:64:ILE:HG21	1:A:88:LYS:HE3	0.62	1.71	4	2
1:A:89:VAL:HG23	1:A:100:VAL:HG12	0.62	1.70	15	1
1:A:89:VAL:HG23	1:A:100:VAL:CG2	0.62	2.25	7	3
1:A:57:LEU:HD13	1:A:95:LEU:HB2	0.62	1.71	18	1
1:A:39:ILE:HD11	1:A:52:ASP:O	0.61	1.94	5	4
1:A:89:VAL:HG12	1:A:106:ALA:HB3	0.61	1.70	17	1
1:A:64:ILE:HG23	1:A:84:ILE:CG2	0.61	2.26	16	10
1:A:61:ARG:HA	1:A:64:ILE:HD12	0.61	1.73	16	2
1:A:30:PHE:CE1	1:A:86:THR:HG23	0.61	2.31	13	6
1:A:39:ILE:HD12	2:A:201:MYR:C14	0.60	2.27	5	5
1:A:30:PHE:CE2	1:A:86:THR:HG23	0.60	2.31	15	5
1:A:81:ASP:HA	1:A:84:ILE:HD12	0.60	1.72	4	10
1:A:60:LEU:CD2	2:A:201:MYR:H141	0.60	2.27	20	1
1:A:85:VAL:O	1:A:89:VAL:HG23	0.60	1.96	12	6
1:A:71:ARG:CB	1:A:80:ILE:HG21	0.60	2.25	16	3
1:A:35:PHE:CE1	1:A:39:ILE:HD11	0.60	2.31	12	3
1:A:92:VAL:HG22	1:A:98:MET:CB	0.59	2.28	19	4
1:A:64:ILE:HD13	1:A:88:LYS:HG2	0.59	1.74	2	3
1:A:67:LEU:HD11	1:A:84:ILE:CG1	0.59	2.28	13	1
1:A:35:PHE:CZ	2:A:201:MYR:H142	0.59	2.31	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:HD12	2:A:201:MYR:H61	0.58	1.74	6	1
1:A:80:ILE:HG22	1:A:84:ILE:CD1	0.58	2.28	9	3
1:A:60:LEU:HD13	1:A:91:ALA:CB	0.58	2.28	4	6
1:A:36:ARG:HA	1:A:39:ILE:HD12	0.58	1.75	16	2
1:A:67:LEU:HD12	1:A:80:ILE:CG2	0.58	2.29	3	1
1:A:21:VAL:HG22	1:A:30:PHE:CD2	0.57	2.34	6	2
1:A:64:ILE:HD11	1:A:87:LEU:HB2	0.57	1.75	5	4
1:A:84:ILE:HG22	1:A:88:LYS:HD2	0.57	1.76	17	2
1:A:85:VAL:CG1	1:A:103:ALA:HB1	0.57	2.30	17	5
1:A:63:VAL:HG23	1:A:87:LEU:HD13	0.57	1.74	20	1
1:A:42:ALA:O	1:A:67:LEU:HD21	0.56	2.00	14	1
1:A:89:VAL:HG22	1:A:106:ALA:CB	0.56	2.30	10	6
1:A:57:LEU:HD12	1:A:95:LEU:CB	0.56	2.30	4	3
1:A:21:VAL:HG22	1:A:30:PHE:CE2	0.56	2.36	4	3
1:A:64:ILE:HD13	1:A:88:LYS:CD	0.56	2.31	16	2
1:A:53:ILE:HD12	2:A:201:MYR:C8	0.56	2.31	8	1
1:A:100:VAL:CG2	1:A:106:ALA:HB2	0.56	2.28	7	1
1:A:56:THR:O	1:A:60:LEU:HD12	0.56	2.01	13	2
1:A:39:ILE:HD12	2:A:201:MYR:C13	0.55	2.30	5	2
1:A:64:ILE:HD12	1:A:84:ILE:HG23	0.55	1.77	17	2
1:A:21:VAL:HG13	1:A:30:PHE:CE1	0.55	2.37	14	1
1:A:19:VAL:HG11	1:A:89:VAL:HG11	0.55	1.78	11	3
1:A:57:LEU:HD23	1:A:95:LEU:HB2	0.55	1.79	3	2
1:A:67:LEU:HD22	1:A:80:ILE:HG23	0.55	1.79	11	1
1:A:77:SER:HB3	1:A:80:ILE:HD12	0.54	1.79	20	7
1:A:89:VAL:HG12	1:A:106:ALA:CB	0.54	2.31	17	1
1:A:84:ILE:HG22	1:A:88:LYS:HE2	0.54	1.79	1	1
1:A:42:ALA:HA	1:A:67:LEU:HD22	0.54	1.79	18	2
1:A:42:ALA:HA	1:A:67:LEU:HD21	0.54	1.79	19	3
1:A:53:ILE:HD12	2:A:201:MYR:H82	0.54	1.80	9	2
1:A:89:VAL:HG23	1:A:100:VAL:CG1	0.54	2.33	15	1
1:A:67:LEU:HD11	1:A:80:ILE:HD12	0.54	1.77	18	1
1:A:42:ALA:O	1:A:46:THR:HG23	0.53	2.03	7	6
1:A:100:VAL:CG1	1:A:106:ALA:HB2	0.53	2.34	17	2
1:A:67:LEU:HD11	1:A:80:ILE:HG23	0.53	1.81	4	1
1:A:60:LEU:HD22	1:A:87:LEU:O	0.53	2.03	13	3
1:A:60:LEU:HD22	1:A:91:ALA:HB2	0.52	1.80	8	4
1:A:100:VAL:HG11	1:A:106:ALA:CB	0.52	2.34	12	1
1:A:19:VAL:CG1	1:A:89:VAL:HG21	0.52	2.34	1	2
1:A:57:LEU:HD23	1:A:95:LEU:CB	0.52	2.33	12	1
1:A:39:ILE:HD11	1:A:54:PRO:HD2	0.52	1.82	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD11	2:A:201:MYR:H142	0.52	1.80	15	2
1:A:77:SER:CB	1:A:80:ILE:HD12	0.52	2.35	7	6
1:A:85:VAL:O	1:A:89:VAL:HG12	0.52	2.05	13	2
1:A:85:VAL:HG22	1:A:103:ALA:HB1	0.51	1.82	8	1
1:A:85:VAL:HG12	1:A:107:GLU:CB	0.51	2.35	12	1
1:A:64:ILE:HD13	1:A:88:LYS:HD2	0.51	1.81	19	1
1:A:39:ILE:HG12	2:A:201:MYR:H141	0.51	1.82	2	1
1:A:81:ASP:O	1:A:85:VAL:HG23	0.51	2.06	16	4
1:A:12:ALA:HB1	1:A:90:PHE:CE1	0.51	2.41	13	1
1:A:85:VAL:HG22	1:A:107:GLU:OE1	0.50	2.07	6	1
1:A:64:ILE:HD13	1:A:88:LYS:HD3	0.50	1.81	16	1
1:A:85:VAL:HB	1:A:103:ALA:HB1	0.50	1.84	13	1
1:A:57:LEU:CD1	1:A:96:LEU:HD23	0.50	2.36	15	1
1:A:85:VAL:HG12	1:A:107:GLU:HB2	0.49	1.84	12	1
1:A:63:VAL:CG2	1:A:87:LEU:HD13	0.49	2.37	20	1
1:A:60:LEU:HD11	2:A:201:MYR:C14	0.49	2.38	10	2
1:A:64:ILE:HD13	1:A:88:LYS:CG	0.49	2.38	20	2
1:A:60:LEU:HD13	1:A:91:ALA:HB1	0.48	1.84	19	1
1:A:46:THR:HG23	1:A:67:LEU:HD13	0.48	1.86	6	1
1:A:67:LEU:HD11	1:A:80:ILE:CD1	0.47	2.39	18	1
1:A:89:VAL:HG13	1:A:100:VAL:CG2	0.47	2.40	20	1
1:A:54:PRO:HG2	2:A:201:MYR:H142	0.47	1.84	6	1
1:A:77:SER:CB	1:A:80:ILE:HG22	0.47	2.39	6	1
1:A:35:PHE:CE2	1:A:39:ILE:HD11	0.47	2.45	16	2
1:A:35:PHE:CE1	2:A:201:MYR:H142	0.47	2.45	16	1
1:A:89:VAL:HA	1:A:106:ALA:HB1	0.47	1.87	19	1
1:A:53:ILE:HG21	2:A:201:MYR:H61	0.46	1.87	2	1
1:A:46:THR:HG23	1:A:67:LEU:CD2	0.46	2.39	3	1
1:A:57:LEU:O	1:A:57:LEU:HD13	0.46	2.10	12	3
1:A:42:ALA:HB1	1:A:67:LEU:HD21	0.46	1.87	15	1
1:A:57:LEU:HA	1:A:60:LEU:HD12	0.46	1.87	19	1
1:A:90:PHE:CE1	2:A:201:MYR:H143	0.46	2.46	15	1
1:A:42:ALA:CB	1:A:67:LEU:HD11	0.46	2.40	20	1
1:A:59:GLN:OE1	1:A:60:LEU:HD22	0.46	2.10	11	1
1:A:39:ILE:HD12	2:A:201:MYR:H132	0.46	1.87	15	1
1:A:93:ALA:HB2	1:A:100:VAL:HG23	0.45	1.88	10	1
1:A:90:PHE:CE1	2:A:201:MYR:H142	0.45	2.46	20	2
1:A:57:LEU:HD13	1:A:95:LEU:CB	0.45	2.40	18	1
1:A:89:VAL:HG13	1:A:100:VAL:HG22	0.45	1.88	20	1
1:A:45:SER:HB3	1:A:67:LEU:HD13	0.45	1.88	2	1
1:A:39:ILE:CD1	2:A:201:MYR:H143	0.44	2.37	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ARG:HE	1:A:80:ILE:HD13	0.43	1.73	6	1
1:A:57:LEU:HD12	1:A:95:LEU:HB3	0.43	1.89	4	1
1:A:63:VAL:HG11	1:A:87:LEU:HD13	0.43	1.89	8	1
1:A:67:LEU:HD23	1:A:84:ILE:CG1	0.43	2.44	1	1
1:A:92:VAL:HG13	1:A:110:TYR:CE1	0.43	2.49	2	1
1:A:85:VAL:HG22	1:A:107:GLU:OE2	0.43	2.13	11	1
1:A:40:ARG:O	1:A:44:VAL:HG23	0.42	2.13	12	1
1:A:54:PRO:O	2:A:201:MYR:H142	0.42	2.14	18	1
1:A:53:ILE:HG21	2:A:201:MYR:H62	0.42	1.90	16	1
1:A:88:LYS:O	1:A:92:VAL:HG23	0.42	2.14	10	1
1:A:53:ILE:HD12	2:A:201:MYR:H81	0.42	1.91	1	1
1:A:90:PHE:CD1	2:A:201:MYR:H143	0.42	2.49	15	1
1:A:64:ILE:HG21	1:A:88:LYS:HZ3	0.42	1.75	5	1
1:A:21:VAL:HG22	1:A:30:PHE:CE1	0.41	2.49	1	2
1:A:92:VAL:HG22	1:A:110:TYR:CD2	0.41	2.50	11	1
1:A:42:ALA:HA	1:A:67:LEU:HD11	0.41	1.90	7	1
1:A:89:VAL:HG23	1:A:100:VAL:CB	0.41	2.46	1	1
1:A:39:ILE:HG22	1:A:87:LEU:CD2	0.41	2.37	8	1
1:A:63:VAL:CG1	1:A:87:LEU:HD13	0.41	2.46	14	1
1:A:21:VAL:HG22	1:A:30:PHE:CG	0.40	2.51	6	1
1:A:89:VAL:HG23	1:A:100:VAL:HG22	0.40	1.93	6	1
1:A:64:ILE:HG21	1:A:88:LYS:NZ	0.40	2.32	8	1
1:A:67:LEU:HD11	1:A:84:ILE:HG12	0.40	1.93	13	1
1:A:84:ILE:HG22	1:A:88:LYS:CE	0.40	2.46	1	1
1:A:42:ALA:HB1	1:A:67:LEU:CD1	0.40	2.46	17	1
1:A:57:LEU:HD12	1:A:95:LEU:HB2	0.40	1.92	4	1
1:A:67:LEU:CD1	1:A:80:ILE:HG23	0.40	2.46	4	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	100/124 (81%)	89±2 (89±2%)	10±2 (10±2%)	1±1 (1±1%)	20	70
All	All	2000/2480 (81%)	1783 (89%)	203 (10%)	14 (1%)	20	70

All 5 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	100	VAL	5
1	A	55	GLU	4
1	A	99	THR	3
1	A	28	LYS	1
1	A	30	PHE	1

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	83/100 (83%)	63±3 (76±4%)	20±3 (24±4%)	2	27
All	All	1660/2000 (83%)	1265 (76%)	395 (24%)	2	27

All 55 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	96	LEU	20
1	A	52	ASP	17
1	A	110	TYR	15
1	A	78	LYS	15
1	A	59	GLN	14
1	A	30	PHE	13
1	A	73	LYS	12
1	A	98	MET	12
1	A	109	MET	12
1	A	57	LEU	11
1	A	82	MET	10
1	A	49	GLU	10
1	A	68	GLN	10
1	A	17	SER	9
1	A	76	SER	9
1	A	29	LYS	9
1	A	28	LYS	9
1	A	107	GLU	9
1	A	41	MET	8

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Mol	Chain	Res	Type	Models (Total)
1	A	88	LYS	8
1	A	101	SER	8
1	A	62	LEU	8
1	A	108	ASN	8
1	A	8	ASP	7
1	A	77	SER	7
1	A	113	MET	7
1	A	11	MET	7
1	A	70	ARG	7
1	A	14	LYS	6
1	A	55	GLU	6
1	A	67	LEU	6
1	A	74	PHE	6
1	A	72	GLU	6
1	A	10	LYS	6
1	A	36	ARG	5
1	A	48	ARG	5
1	A	61	ARG	5
1	A	65	CYS	5
1	A	79	GLU	5
1	A	58	ASP	5
1	A	60	LEU	4
1	A	40	ARG	4
1	A	18	ASN	4
1	A	111	SER	4
1	A	71	ARG	3
1	A	32	GLU	3
1	A	69	GLU	3
1	A	15	ARG	3
1	A	45	SER	2
1	A	46	THR	2
1	A	81	ASP	2
1	A	97	ASN	1
1	A	53	ILE	1
1	A	112	GLN	1
1	A	86	THR	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MYR	A	201	1	13,14,15	0.56±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MYR	A	201	1	12,13,15	0.44±0.00	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	A	201	1	-	0±0,12,12,13	-

There are no bond-length outliers.

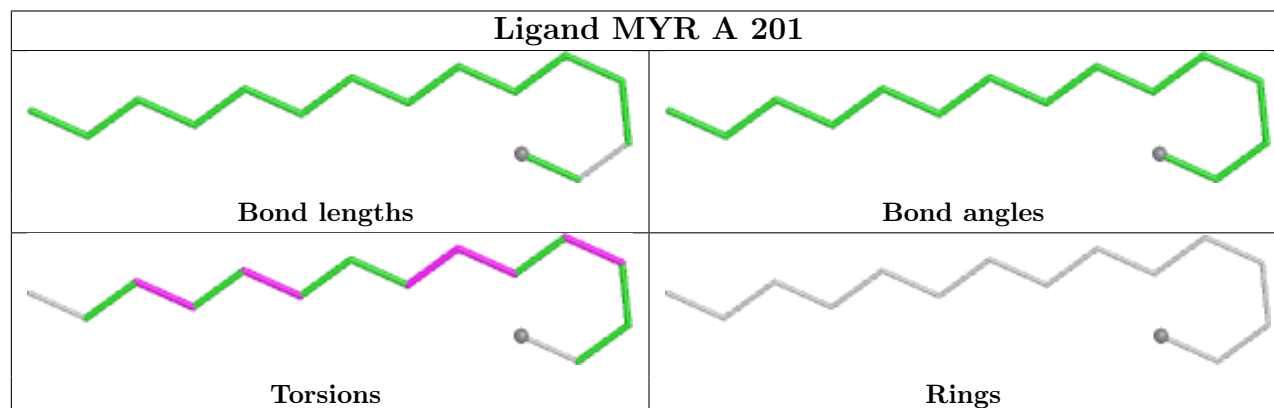
There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 74% 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

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	1166
Number of shifts mapped to atoms	1166
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	113	-1.31 ± 0.11	Should be checked
$^{13}\text{C}_\beta$	101	-0.41 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	112	2.34 ± 0.12	Should be applied
^{15}N	103	0.93 ± 0.48	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1066 atoms were assigned a chemical shift out of a possible 1372. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	486/502 (97%)	195/204 (96%)	199/200 (100%)	92/98 (94%)
Sidechain	536/797 (67%)	338/519 (65%)	190/242 (79%)	8/36 (22%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	44/73 (60%)	23/36 (64%)	19/35 (54%)	2/2 (100%)
Overall	1066/1372 (78%)	556/759 (73%)	408/477 (86%)	102/136 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1165 atoms were assigned a chemical shift out of a possible 1578. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	545/597 (91%)	217/246 (88%)	225/236 (95%)	103/115 (90%)
Sidechain	576/908 (63%)	362/589 (61%)	205/274 (75%)	9/45 (20%)
Aromatic	44/73 (60%)	23/36 (64%)	19/35 (54%)	2/2 (100%)
Overall	1165/1578 (74%)	602/871 (69%)	449/545 (82%)	114/162 (70%)

7.1.4 Statistically unusual chemical shifts [i](#)

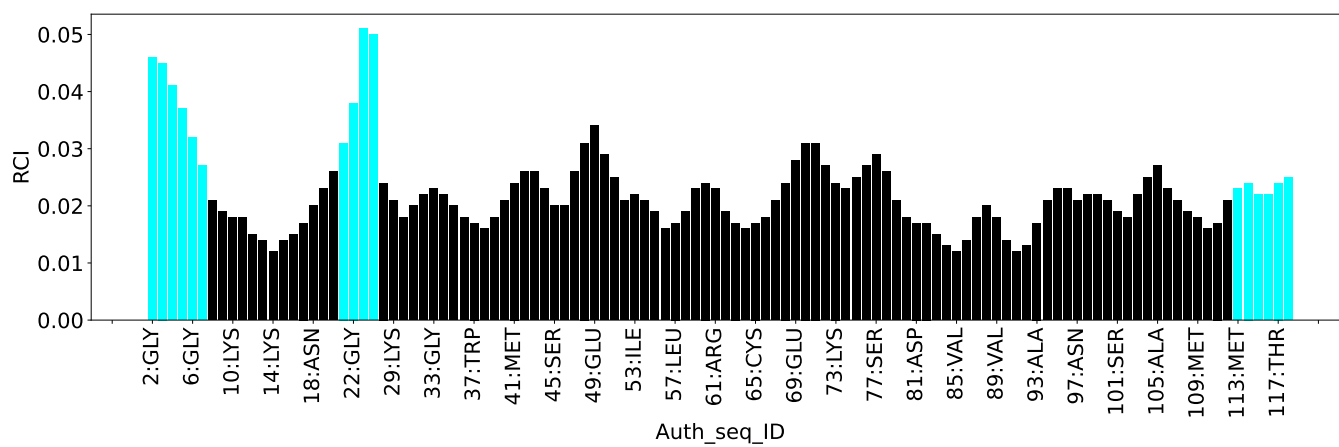
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	48	ARG	CB	19.14	21.74 – 39.52	-6.5
1	A	64	ILE	CG1	18.49	19.24 – 36.26	-5.4

7.1.5 Random Coil Index (RCI) plots [i](#)

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 [i](#)

8.1 Conformationally restricting restraints [i](#)

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	456
Intra-residue ($ i-j =0$)	1
Sequential ($ i-j =1$)	97
Medium range ($ i-j >1$ and $ i-j <5$)	237
Long range ($ i-j \geq 5$)	114
Inter-chain	7
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	3.6
Number of long range restraints per residue ¹	0.9

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 [i](#)

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 [i](#)

Distance violations less than 0.1 Å are not included in the calculation. There are no distance violations

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

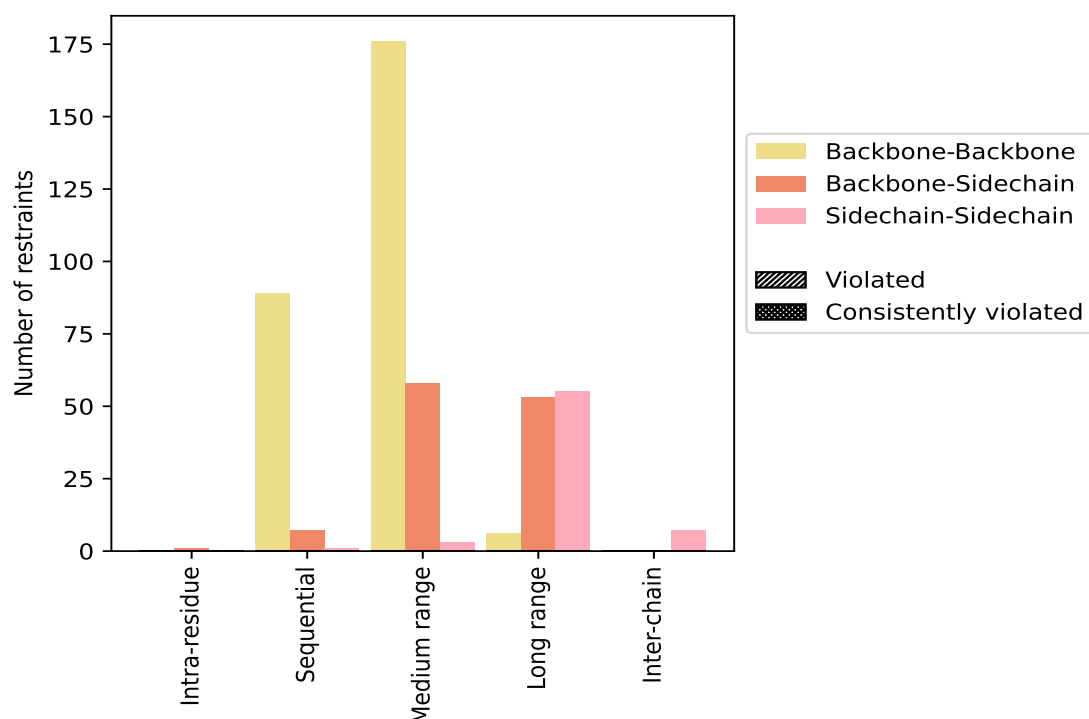
9.1 Summary of distance violations

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 ($i-j =0$)	1	0.2	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	1	0.2	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
Sequential ($i-j =1$)	97	21.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	89	19.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	1.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	0.2	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	237	52.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	176	38.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	58	12.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	3	0.7	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	114	25.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	6	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	53	11.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	55	12.1	0	0.0	0.0	0	0.0	0.0
Inter-chain	7	1.5	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	7	1.5	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	456	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	271	59.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	119	26.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	66	14.5	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 disulfide bonds are counted in their appropriate category on the x-axis

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

No violations found

9.3 Distance violation statistics for the ensemble [i](#)

No violations found

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

No violations found

9.5 All violated distance restraints [i](#)

No violations found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found