

Full wwPDB NMR Structure Validation Report (i)

Jan 29, 2024 – 11:14 pm GMT

PDB ID : 8CA0 BMRB ID : 34783

Title: Macrophage inhibitory factor (MIF) in complex with small molecule PAV174

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Deposited on : 2023-01-24

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 (i) 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 : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

wwPDB-RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

wwPDB-ShiftChecker : v1.2

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

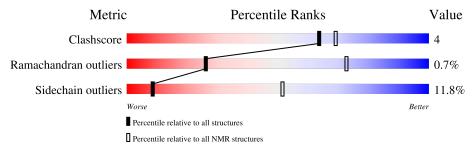
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment is 1%.

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 $(\# \mathrm{Entries})$	$rac{ m NMR~archive}{ m (\#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 <=5%

Mol	Chain	Length	Quality of chain	
1	A	114	87%	13%
1	В	114	89%	10% •
1	С	114	91%	9%



2 Ensemble composition and analysis (i)

This entry contains 4 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:1-A:114, B:1-B:114, C:1-	0.76	3			
	C:114 (342)					

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4



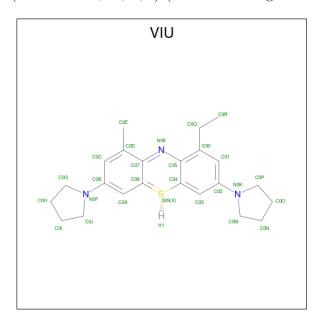
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5221 atoms, of which 2596 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Macrophage migration inhibitory factor.

Mol	Chain	Residues		Atoms					Trace
1	Λ	114	Total	С	Н	N	О	S	0
1	A	114	1722	548	856	151	161	6	U
1	В	114	Total	С	Н	N	О	S	0
1	Б	114	1722	548	856	151	161	6	U
1	С	114	Total	С	Н	N	О	S	0
1		114	1722	548	856	151	161	6	U

• Molecule 2 is 1-ethyl-9-methyl-3,7-dipyrrolidin-1-yl-phenothiazine (three-letter code: VIU) (formula: C₂₃H₂₉N₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				
2	Λ	1	Total	С	Н	N	S
2	А	1	55	23	28	3	1

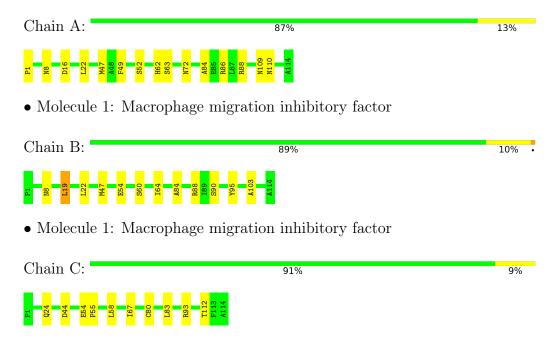


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Macrophage migration inhibitory factor

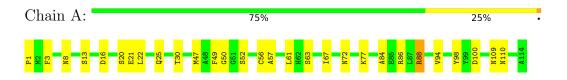


4.2 Scores per residue for each member of the ensemble

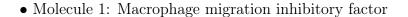
Colouring as in section 4.1 above.

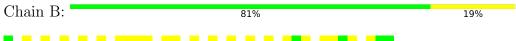
4.2.1 Score per residue for model 1

• Molecule 1: Macrophage migration inhibitory factor











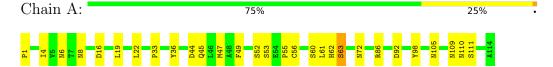
• Molecule 1: Macrophage migration inhibitory factor



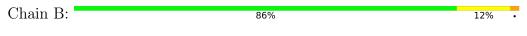


4.2.2 Score per residue for model 2

• Molecule 1: Macrophage migration inhibitory factor



• Molecule 1: Macrophage migration inhibitory factor





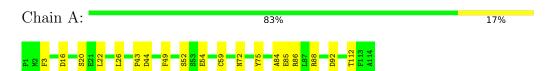
• Molecule 1: Macrophage migration inhibitory factor





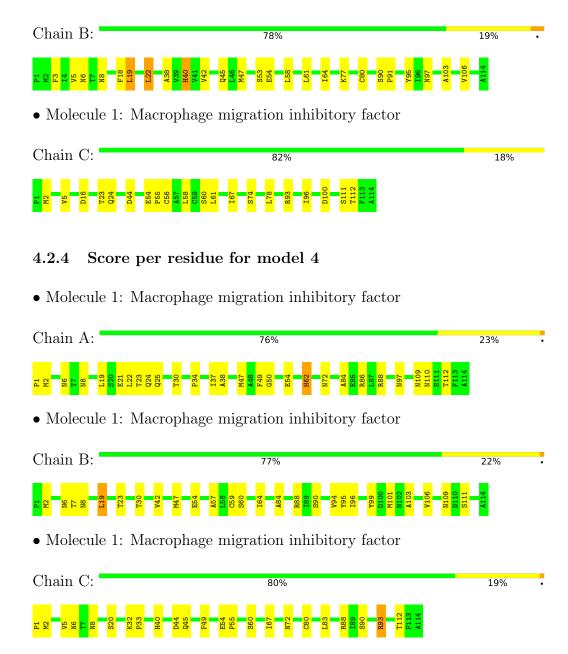
4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Macrophage migration inhibitory factor



• Molecule 1: Macrophage migration inhibitory factor







Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing.

Of the 4 calculated structures, 4 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	structure calculation	
HADDOCK	refinement	

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	85
Number of shifts mapped to atoms	85
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%



6 Model quality (i)

6.1 Standard geometry (i)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	866	856	858	10±3
1	В	866	856	858	10±2
1	С	866	856	858	8±3
2	A	27	28	0	0±0
All	All	10500	10384	10296	90

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:C:5:VAL:HG12	1:C:60:SER:H	0.63	1.54	3	2
1:B:3:PHE:HA	1:C:2:MET:HB3	0.60	1.73	3	1
1:B:19:LEU:HD13	1:B:19:LEU:H	0.60	1.56	3	3
1:A:110:ASN:HA	1:C:80:CYS:SG	0.60	2.37	1	3
1:B:47:MET:HB3	1:C:40:HIS:HD2	0.59	1.57	1	1
1:A:1:PRO:HG3	1:A:30:THR:HG21	0.59	1.75	4	2
1:A:49:PHE:HD1	1:B:38:ALA:HB2	0.59	1.58	3	1
1:B:6:ASN:ND2	1:B:42:VAL:HB	0.58	2.13	4	2
1:A:50:GLY:HA2	1:B:23:THR:HG21	0.58	1.74	4	1



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Atom-1	Atom-2	Clash(Å)	$Distance(\mathring{A})$	Mod	
		` ′	, ,	Worst	Total
1:B:60:SER:HB3	1:B:99:TYR:HE2	0.57	1.59	4	2
1:A:49:PHE:CD1	1:B:38:ALA:HB2	0.56	2.35	3	1
1:B:8:ASN:HB3	1:B:47:MET:HG2	0.55	1.77	4	2
1:A:2:MET:HB3	1:A:62:HIS:HB2	0.55	1.79	4	1
1:B:64:ILE:HD11	1:B:103:ALA:HA	0.54	1.79	3	3
1:A:6:ASN:HD21	1:A:45:GLN:HG3	0.53	1.63	2	1
1:A:1:PRO:HB3	1:A:63:SER:HB3	0.53	1.80	2	2
1:A:84:ALA:O	1:A:88:ARG:HA	0.53	2.03	1	3
1:A:8:ASN:HB3	1:A:47:MET:HG2	0.53	1.80	4	3
1:B:91:PRO:HB2	1:C:109:ASN:HA	0.52	1.79	2	1
1:A:112:THR:HB	1:C:72:ASN:HB3	0.52	1.81	4	1
1:C:6:ASN:HB2	1:C:58:LEU:HD21	0.52	1.80	2	1
1:A:3:PHE:HD1	1:A:61:LEU:HG	0.52	1.65	1	1
1:B:7:THR:HA	1:B:47:MET:SD	0.52	2.45	4	1
1:B:36:TYR:HA	1:B:108:TRP:HZ3	0.51	1.66	2	1
1:A:49:PHE:HB3	1:A:54:GLU:HB2	0.50	1.83	3	2
1:A:4:ILE:HG23	1:A:60:SER:HB2	0.50	1.84	2	1
1:B:60:SER:HB3	1:B:99:TYR:CE2	0.50	2.42	4	2
1:A:8:ASN:OD1	1:A:55:PRO:HA	0.49	2.08	2	1
1:C:8:ASN:HA	1:C:45:GLN:O	0.48	2.08	1	2
1:A:2:MET:HB2	2:A:201:VIU:C0N	0.48	2.38	4	1
1:C:82:LEU:O	1:C:86:ARG:HB2	0.48	2.09	1	1
1:A:112:THR:HA	1:C:96:ILE:O	0.47	2.08	3	1
1:B:6:ASN:HB3	1:B:45:GLN:HG3	0.47	1.85	3	1
1:A:57:ALA:HB3	1:A:94:VAL:HG22	0.47	1.85	1	1
1:C:96:ILE:HG22	1:C:97:ASN:H	0.47	1.70	1	1
1:B:102:ASN:HB2	1:B:105:ASN:HB2	0.46	1.86	1	1
1:B:57:ALA:O	1:B:94:VAL:HA	0.46	2.10	4	1
1:C:8:ASN:HB3	1:C:55:PRO:HA	0.46	1.88	4	1
1:B:8:ASN:OD1	1:B:55:PRO:HA	0.46	2.10	1	1
1:A:50:GLY:HA2	1:B:34:PRO:O	0.45	2.11	1	1
1:B:47:MET:HB3	1:C:40:HIS:CD2	0.45	2.44	1	1
1:B:80:CYS:HB2	1:C:110:ASN:OD1	0.45	2.12	1	1
1:A:97:ASN:HD21	1:C:1:PRO:HG3	0.45	1.72	4	1
1:C:83:LEU:HB3	1:C:89:ILE:HD11	0.44	1.88	2	2
1:B:18:PHE:O	1:B:22:LEU:HB2	0.44	2.12	3	1
1:B:80:CYS:HB3	1:B:91:PRO:HB3	0.44	1.88	3	1
1:A:21:GLU:O	1:A:25:GLN:HG2	0.44	2.11	4	2
1:A:8:ASN:HB3	1:A:47:MET:CG	0.44	2.42	2	1
1:B:6:ASN:HB2	1:C:40:HIS:CE1	0.44	2.48	4	1
1:A:38:ALA:HB2	1:C:49:PHE:HD2	0.43	1.73	4	1
	l.	l.			1



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Atom-1	Atom-2	Clash(Å)	$\operatorname{Distance}(\mathring{\mathrm{A}})$	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:5:VAL:HB	1:B:40:HIS:O	0.43	2.12	3	1
1:B:84:ALA:O	1:B:88:ARG:HA	0.43	2.14	1	3
1:B:59:CYS:SG	1:B:96:ILE:HG12	0.43	2.54	4	1
1:B:77:LYS:HA	1:C:110:ASN:OD1	0.42	2.14	1	1
1:A:3:PHE:HE1	1:A:59:CYS:HB3	0.42	1.74	3	1
1:C:32:LYS:HE2	1:C:33:PRO:HD2	0.42	1.90	4	1
1:A:23:THR:HA	1:A:37:ILE:HG21	0.42	1.91	4	1
1:A:33:PRO:HG2	1:A:36:TYR:HD1	0.42	1.75	2	1
1:C:91:PRO:HA	1:C:94:VAL:CG2	0.42	2.44	2	1
1:B:2:MET:O	1:C:2:MET:HG3	0.42	2.14	4	1
1:B:9:VAL:O	1:B:43:PRO:HB2	0.41	2.15	2	1
1:A:34:PRO:HA	1:A:37:ILE:CG1	0.41	2.46	4	1
1:B:36:TYR:HA	1:B:108:TRP:CZ3	0.41	2.50	2	1
1:C:93:ARG:O	1:C:93:ARG:HD2	0.40	2.16	4	1
1:C:104:ALA:HA	1:C:114:ALA:HB2	0.40	1.93	1	1
1:A:47:MET:SD	1:A:56:CYS:HB2	0.40	2.56	2	1
1:C:91:PRO:HA	1:C:94:VAL:HG23	0.40	1.92	2	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	$112/114\ (98\%)$	107±1 (96±1%)	4±1 (4±1%)	1±0 (1±0%)	2	1	69
1	В	112/114 (98%)	103±2 (92±2%)	8±2 (8±2%)	1±0 (1±0%)	2	6	73
1	С	112/114~(98%)	105±3 (94±3%)	7±3 (6±3%)	0±0 (0±0%)	3	8	78
All	All	1344/1368 (98%)	1258 (94%)	77 (6%)	9 (1%)	2	6	73

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	109	ASN	3
1	С	55	PRO	2



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Mol	Chain	Res	Type	Models (Total)
1	В	108	TRP	1
1	A	43	PRO	1
1	В	106	VAL	1
1	В	109	ASN	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	94/94~(100%)	82±3 (87±4%)	12±3 (13±4%)	7 49		
1	В	94/94~(100%)	85±2 (90±2%)	9±2 (10±2%)	12 58		
1	С	94/94 (100%)	82±2 (87±2%)	12±2 (13±2%)	7 48		
All	All	1128/1128 (100%)	995 (88%)	133 (12%)	8 51		

All 77 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	22	LEU	4
1	A	72	ASN	4
1	A	86	ARG	4
1	В	19	LEU	4
1	С	54	GLU	4
1	С	67	ILE	4
1	С	93	ARG	4
1	С	112	THR	4
1	A	16	ASP	3
1	A	52	SER	3
1	В	54	GLU	3
1	В	90	SER	3
1	С	24	GLN	3
1	В	95	TYR	3
1	С	44	ASP	3
1	A	20	SER	2
1	A	49	PHE	2
1	A	98	TYR	2
1	В	16	ASP	2



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Mol	nued fron Chain	m Res	Type	Models (Total)
1	В	53	SER	2
1	В	61	LEU	2
1	В	73	ARG	2
1	В	112	THR	2
1	C	23	THR	2
1	A	19	LEU	2
1	A	44	ASP	2
1	A	62	HIS	2
1	A	92	ASP	2
1	В	22	LEU	2
1	C	16	ASP	2
1	C	20	SER	2
1	C	58	LEU	2
1	C	100	ASP	2
1	A	13	SER	1
1	A	56	CYS	1
1	A	67	ILE	1
1	A	77	LYS	1
1	A	88	ARG	1
1	A	100	ASP	1
1	В	52	SER	1
1	В	60	SER	1
1	C	3	PHE	1
1	C	36	TYR	1
1	C	53	SER	1
1	C	97	ASN	1
1	A	53	SER	1
1	A	61	LEU	1
1	A	63	SER	1
1	A	105	ASN	1
1	A	111	SER	1
1	В	20	SER	1
1	С	26	LEU	1
1	С	52	SER	1
1	С	71	GLN	1
1	С	92	ASP	1
1	A	26	LEU	1
1	A	75	TYR	1
1	A	85	GLU	1
1	В	40	HIS	1
1	В	58	LEU	1
1	В	77	LYS	1



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Mol	Chain	Res	Type	Models (Total)
1	В	97	ASN	1
1	С	56	CYS	1
1	С	61	LEU	1
1	С	74	SER	1
1	С	78	LEU	1
1	С	111	SER	1
1	A	6	ASN	1
1	A	24	GLN	1
1	В	30	THR	1
1	В	101	MET	1
1	В	106	VAL	1
1	В	111	SER	1
1	С	6	ASN	1
1	С	83	LEU	1
1	С	88	ARG	1
1	С	90	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

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.



Mal	Tuno	Chain	Dec	Link		Bond leng	gths
MOI	туре	Chain	nes		Counts	RMSZ	#Z>2
2	VIU	A	201	-	29,31,31	1.42 ± 0.02	3±0 (9±1%)

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.

Mal	Type	Chain	Pos	Link		Bond an	gles
IVIOI	туре	Chain	ites	LIIIK	Counts	RMSZ	#Z>2
2	VIU	A	201	-	32,45,45	1.36 ± 0.01	5±0 (15±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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VIU	A	201	-	-	$0\pm0,10,32,32$	$0\pm0,4,5,5$

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Chain	Dag	Trino	Atoma	7	Observed(Å)	Ideal(Å)	Mod	dels
Mol	Chain	nes	Type	Atoms	L	Observed(A)	ideai(A)	Worst	Total
2	A	201	VIU	C07-N06	5.25	1.40	1.30	1	4
2	A	201	VIU	C07-C0D	3.91	1.39	1.47	1	4
2	A	201	VIU	C02-N0K	2.08	1.33	1.38	1	3

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Chain Res Type Atoms Z		7	Observed(0)	$Ideal(^{o})$	Models		
MIOI	Chain	nes	туре	Atoms	L	$Observed(^o)$	ideai()	Worst	Total
2	A	201	VIU	C05-N06-C07	4.49	124.87	117.89	4	4
2	A	201	VIU	C0O-C0N-C0M	2.09	99.29	105.19	2	4
2	A	201	VIU	C0N-C0O-C0P	2.08	99.30	105.19	2	4
2	A	201	VIU	C0H-C0I-C0J	2.07	99.35	105.19	1	4
2	A	201	VIU	C0I-C0H-C0G	2.06	99.37	105.19	3	4

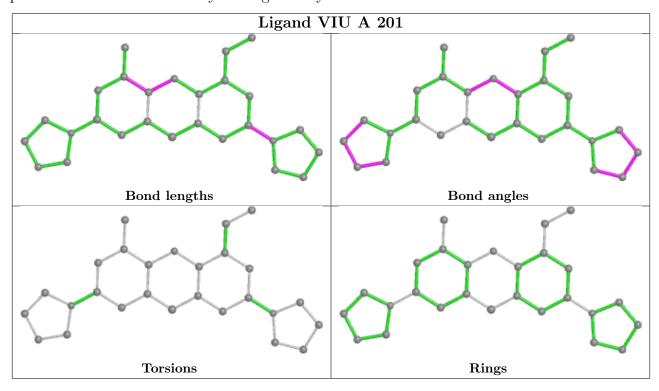


There are no chirality outliers.

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 then 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 (i)

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% 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	85
Number of shifts mapped to atoms	85
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 1%, i.e. 57 atoms were assigned a chemical shift out of a possible 4506. 0 out of 57 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/1689~(0%)	0/687 (0%)	0/684 (0%)	0/318 (0%)
Sidechain	18/2484 (1%)	18/1632 (1%)	0/756~(0%)	0/96~(0%)
Aromatic	39/333 (12%)	39/162 (24%)	0/162 (0%)	0/9 (0%)
Overall	57/4506 (1%)	57/2481 (2%)	0/1602 (0%)	0/423~(0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 57 atoms were assigned a chemical shift out of a possible 4506. 0 out of 57 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/1689 (0%)	0/687 (0%)	0/684 (0%)	0/318 (0%)
Sidechain	18/2484 (1%)	18/1632 (1%)	0/756 (0%)	0/96 (0%)
Aromatic	39/333 (12%)	39/162 (24%)	0/162 (0%)	0/9 (0%)
Overall	57/4506 (1%)	57/2481 (2%)	0/1602 (0%)	0/423~(0%)

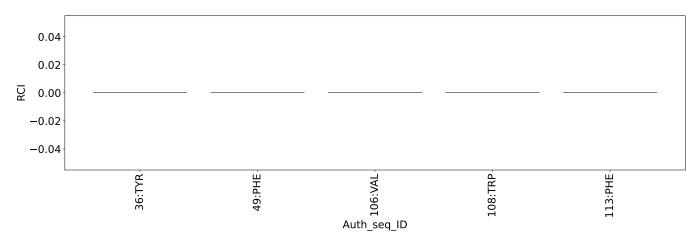
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

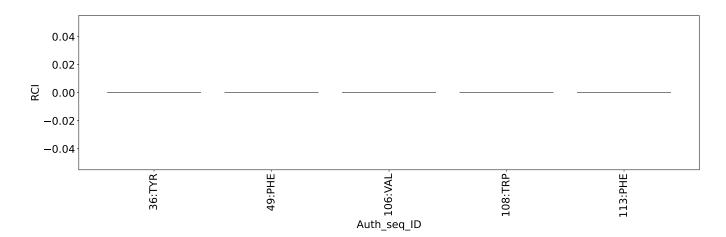
The image below reports random coil index values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted 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:



Random coil index (RCI) for chain B:





Random coil index (RCI) for chain C:

