

Full wwPDB NMR Structure Validation Report (i)

Mar 2, 2022 – 04:05 PM EST

PDB ID	:	6VXG
Title	:	Structure of the C-terminal Domain of RAGE and Its Inhibitor
Authors	:	Ramirez, L.; Shekhtman, A.
Deposited on	:	2020-02-21

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 following versions of software and data (see references (1)) were used in the production of this report:

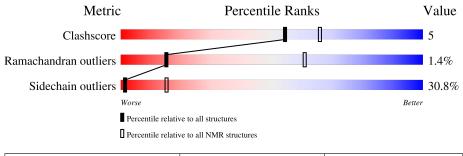
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 60%.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} \; { m archive} \ (\#{ m Entries})$					
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	А	43	23%	12%	•	63%						



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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	Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model										
1	A:2-A:16 (15)	0.30	6								

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 5 single-model clusters were found.

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



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 344 atoms, of which 168 are hydrogens and 0 are deuteriums.

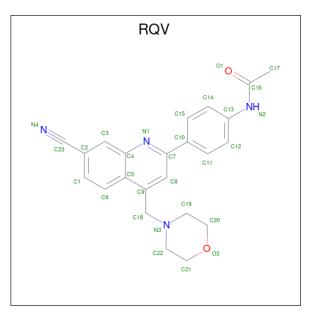
• Molecule 1 is a protein called Advanced glycosylation end product-specific receptor.

Mol	Chain	Residues		Atoms										
1	٨	16	Total	С	Η	Ν	Ο	S	0					
1	A	16	293	87	146	35	24	1	0					

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP Q15109

• Molecule 2 is N-(4-{7-cyano-4-[(morpholin-4-yl)methyl]quinolin-2-yl}phenyl)acetam ide (three-letter code: RQV) (formula: $C_{23}H_{22}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						
0	٨	1	Total	С	Η	Ν	0		
	А		51	23	22	4	2		

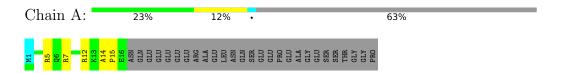


4 Residue-property plots (i)

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: Advanced glycosylation end product-specific receptor



4.2 Scores per residue for each member of the ensemble

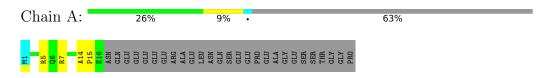
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Advanced glycosylation end product-specific receptor



4.2.2 Score per residue for model 2





4.2.3 Score per residue for model 3

• Molecule 1: Advanced glycosylation end product-specific receptor



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4.2.4 Score per residue for model 4

• Molecule 1: Advanced glycosylation end product-specific receptor

Ch	naiı	n .	A:		14	1%			21	L%		•									63%)					
M1	R5 Q6	R7	R8	R12 K13	A14	E16	ASN GLU GLU	GLU GLU	GLU GLU	ALA	GLU	ASN GLN	SER	GLU PRO	GLU	ALA GLY	GLU SER	SER	A TO	PRO							

4.2.5 Score per residue for model 5

• Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:	19%	14% ••	63%
M1 W2 R4 R5 R6 R6 R7	R12 K13 A14 A14 A14 A14 A15 A15 A15 A15 A10 GLU	GLU GLU GLU GLU GLU CLU CLU CLU GLU GLU GLU	PRO GLU GLU GLU SER SER SER SER CLU GLY GLY

4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:	23%	9% • •	63%
M1 R4 R7 R12 R13 R13 F15 F16 E16	ASN GLU GLU GLU GLU GLU GLU ARG	ALA GLU LEU ASN ASN CLU CLU CLU CLU CLU CLU CLU SER SER SER SER CLU CLU CLU CLU CLU CLU CLU CLU	

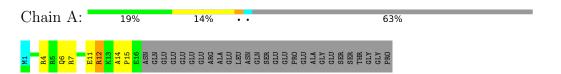
4.2.7 Score per residue for model 7

Chain A.	26%	9% •	63%	
	2076	970 •	05/8	
M1 R5 Q6 R7 K13 K13	ASN 35LN 35LU 35LU 35LU 35LU 35LU 35LU 37LA AALA	LEU ASN GLU CLU CLU CLU CLU CLU CLU CLU CLU	PRO	
M1 R5 R7 K13 F16	ASN GLU GLU GLU GLU GLU GLU ARG	LEU ASN GLN SER GLU GLU PRO GLU GLU GLU GLU	SER THR GLY GLY PRO	



4.2.8 Score per residue for model 8

• Molecule 1: Advanced glycosylation end product-specific receptor



4.2.9 Score per residue for model 9

• Molecule 1: Advanced glycosylation end product-specific receptor



4.2.10 Score per residue for model 10

• Molecule 1: Advanced glycosylation end product-specific receptor

Chain	A:		26%	9%	•		63%	
M1 W2 R7	A14 P15	E16 ASN GLU GLU GLU	GLU GLU GLU ALA ALA CLU CLU CLU	SER GLU GLU	PRO GLU ALA GLY GLY SER SER	THR GLY GLY PRO		

4.2.11 Score per residue for model 11

• Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:	21%	14%	•	63%
M1 W2 W2 R4 R5 Q6 Q6 Q6 R12 K13 K13	P15 E16 ASN GLU GLU GLU GLU	GLU ARG ALA GLU LEU ASN	GLN SER GLU GLU GLU GLU GLY GLV SER SER SER SER SER SER SER SER	

4.2.12 Score per residue for model 12

Chain A:	23%	12% •	63%	
M1 R5 Q6 R7 R12 R13 A14 A14	E16 ASN GLN GLU GLU GLU GLU GLU	ARC ALA ALA ALA ALA ASN ALA CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	CUU SER THR GLY GLY CUY	



4.2.13 Score per residue for model 13

• Molecule 1: Advanced glycosylation end product-specific receptor



4.2.14 Score per residue for model 14

• Molecule 1: Advanced glycosylation end product-specific receptor



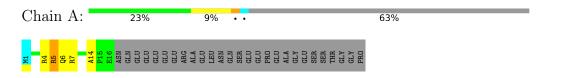
4.2.15 Score per residue for model 15

• Molecule 1: Advanced glycosylation end product-specific receptor

Chain	А	.:			16	%				1	.6%)		•	•												6	3%	, D					
M1 Q6 R7 R7	G9	E10	E11	K13	A14	P15 E16	ASN	GLN	GLU	GLU	GLU	ARG	ALA	GLU	LEU	GLN	SER	GLU	PRO	GLU	ALA	GLY	GLU	SER	THR	GLY	GLY	DN/4						

4.2.16 Score per residue for model 16

• Molecule 1: Advanced glycosylation end product-specific receptor



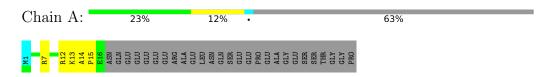
4.2.17 Score per residue for model 17

Chain A:	19%	14% ••	63%	
M1 R4 R5 R7 B11	R12 K13 P16 P15 ASN GLU GLU	GLU GLU GLU GLU GLU ARG AILA ARG CLU LEU CLU SER SER SEL	PR0 CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	



4.2.18 Score per residue for model 18

• Molecule 1: Advanced glycosylation end product-specific receptor



4.2.19 Score per residue for model 19

• Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:	21%	14%	•	63%
M1 R5 Q6 R7 R8	R12 K13 A14 A14 A14 A14 A14 A14 A14 A14 A14 A14	GLU GLU ALA ALA GLU LEU ASN	GLN SER GLU GLU PRO GLV GLY SER SER SER SER SER SER SER SER	

4.2.20 Score per residue for model 20

Chain A:	23%	9% ••	63%	
M1 R4 R7 E10 E11 R12	E16 ASN GLU GLU GLU GLU GLU GLU	ARG ALA ALA GLU CELU SER SER SER GLU GLU GLU	GLU SER SER CLU THR CLY CLY	



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	3.98.5
CYANA	structure calculation	3.98.5

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	383
Number of shifts mapped to atoms	383
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%



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: RQV

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	А	139	137	137	1 ± 1
2	А	29	22	0	1±1
All	All	3360	3180	2740	33

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 5.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Mod	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:A:101:RQV:C9	2:A:101:RQV:C18	1.61	1.74	3	1
1:A:12:ARG:HB2	2:A:101:RQV:N4	0.92	1.80	8	3
2:A:101:RQV:C18	2:A:101:RQV:C5	0.80	2.59	3	1
1:A:13:LYS:HE3	2:A:101:RQV:N4	0.74	1.98	7	1
1:A:12:ARG:CB	2:A:101:RQV:N4	0.69	2.55	8	1
1:A:14:ALA:HB1	1:A:15:PRO:HD2	0.67	1.65	17	16
2:A:101:RQV:C18	2:A:101:RQV:C6	0.59	2.79	3	1
1:A:10:GLU:OE1	1:A:14:ALA:HB3	0.59	1.98	15	1
1:A:4:ARG:HB3	2:A:101:RQV:C18	0.51	2.35	16	1
1:A:12:ARG:HB3	2:A:101:RQV:N4	0.46	2.25	9	1
1:A:10:GLU:CD	1:A:14:ALA:HB3	0.46	2.30	15	1

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:5:ARG:NH2	1:A:14:ALA:H	0.43	2.11	16	1	
1:A:10:GLU:O	1:A:11:GLU:CB	0.43	2.67	15	1	
2:A:101:RQV:C6	2:A:101:RQV:N3	0.42	2.82	19	2	
1:A:10:GLU:O	1:A:11:GLU:HB3	0.40	2.16	20	1	

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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	Analysed Favoured		Outliers	Percentiles		
1	А	14/43~(33%)	$9{\pm}1~(64{\pm}8\%)$	$5\pm1 (35\pm9\%)$	0±0 (1±3%)	15 61		
All	All	280/860~(33%)	179 (64%)	97~(35%)	4 (1%)	15 61		

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	А	11	GLU	2
1	А	12	ARG	1
1	А	10	GLU	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	А	13/36~(36%)	$9\pm1~(69\pm11\%)$	4 ± 1 (31 $\pm11\%$)	1 15		
All	All	260/720~(36%)	180 (69%)	80 (31%)	1 15		

All 11 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	А	7	ARG	19
1	А	12	ARG	12
1	А	5	ARG	11
1	А	6	GLN	10
1	А	4	ARG	8
1	А	13	LYS	5
1	А	2	TRP	4
1	А	8	ARG	4
1	А	11	GLU	4
1	А	16	GLU	2
1	А	3	GLN	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	Turne	Chain	Dec	Tink	Bond lengths			
IVIOI	туре	Unam	nes	LINK	Counts	RMSZ	#Z>2	
2	RQV	А	101	-	32,32,32	$1.88 {\pm} 0.46$	4±1 (11±4%)	

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.

Γ	/[_]	Turne	Chain	Dec	Tiple		gles	
10	Mol	Type	Chain	nes	LIIK	Counts	RMSZ	#Z>2
	2	RQV	А	101	-	42,44,44	3.00 ± 0.99	7±2 (16±3%)

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	RQV	А	101	-	-	$0\pm0,14,22,22$	$0\pm0,4,4,4$

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

Mol	Chain	Res	Tuno	Atoms	Z	Observed(Å)	Ideal(Å)	Mod	dels
	Ullalli	nes	Type	Atoms		Observeu(A)	Iueai(A)	Worst	Total
2	А	101	RQV	C18-N3	10.28	1.67	1.47	20	19
2	А	101	RQV	C18-C9	8.93	1.74	1.52	3	17
2	А	101	RQV	C8-C7	4.86	1.47	1.39	15	1
2	А	101	RQV	C7-N1	4.27	1.26	1.33	15	1
2	А	101	RQV	C9-C5	4.11	1.52	1.42	14	3
2	А	101	RQV	C19-N3	3.53	1.56	1.46	16	1
2	А	101	RQV	C2-C23	3.20	1.37	1.44	7	2
2	А	101	RQV	C4-N1	3.03	1.42	1.37	15	20
2	А	101	RQV	C22-N3	2.95	1.55	1.46	18	4
2	А	101	RQV	C8-C9	2.88	1.42	1.37	5	8

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

Mol	Mol Chain		Type	Atoms	7	$Observed(^{o})$	Ideal(°)	Models	
	Ullalli	Res	Type	Atoms		Observed()	Ideal()	Worst	Total
2	А	101	RQV	C9-C18-N3	29.47	156.21	114.14	6	18
2	А	101	RQV	C18-N3-C22	9.88	89.08	111.06	6	11
2	А	101	RQV	C18-N3-C19	8.27	92.66	111.06	9	10
2	А	101	RQV	C18-C9-C5	7.17	107.41	119.93	6	13
2	А	101	RQV	C7-N1-C4	6.09	122.59	118.06	17	20

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Mol	Chain	Dec	Turne	Atoms	Z	Observed(°)	Ideal(0)	Moo	lels
	Unam	Res	Type	Atoms	2	Observed()	$\mathrm{Ideal}(^{o})$	Worst	Total
2	А	101	RQV	C3-C2-C23	5.88	114.57	119.65	13	14
2	А	101	RQV	C8-C9-C5	4.55	112.66	118.70	20	3
2	А	101	RQV	C7-C8-C9	3.42	124.10	119.98	20	2
2	А	101	RQV	C8-C7-N1	3.18	119.33	122.23	10	19
2	А	101	RQV	C1-C2-C23	3.04	114.92	119.99	6	11
2	А	101	RQV	C22-N3-C19	2.94	102.22	108.83	16	1
2	А	101	RQV	C20-C19-N3	2.65	114.11	110.10	12	2
2	А	101	RQV	C21-C22-N3	2.39	106.48	110.10	11	2
2	А	101	RQV	C11-C10-C7	2.04	118.06	121.28	8	13

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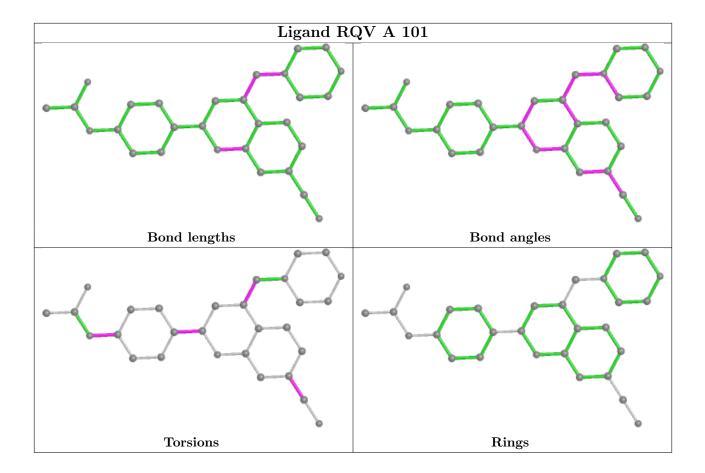
There are no chirality outliers.

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 sufficient 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 60% for the well-defined parts and 60% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: D_1000246866_cs_P1.str.V1

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	383
Number of shifts mapped to atoms	383
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)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	$\textbf{Correction} \pm \textbf{precision}, \textit{ppm}$	Suggested action
$^{13}C_{\alpha}$	40	3.32 ± 0.63	Should be applied
$^{13}C_{\beta}$	36	3.03 ± 0.12	Should be applied
$^{13}C'$	0		None (insufficient data)
¹⁵ N	40	-1.92 ± 0.62	Should be applied

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 60%, i.e. 145 atoms were assigned a chemical shift out of a possible 243. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	55/73~(75%)	27/29~(93%)	14/30~(47%)	14/14~(100%)
Sidechain	90/158~(57%)	59/96~(61%)	31/44~(70%)	0/18~(0%)

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	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Aromatic	0/12~(0%)	0/6~(0%)	0/5~(0%)	0/1~(0%)
Overall	145/243~(60%)	86/131 (66%)	45/79~(57%)	14/33 (42%)

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 153 atoms were assigned a chemical shift out of a possible 256. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N
Backbone	58/78~(74%)	28/31~(90%)	15/32~(47%)	15/15~(100%)
Sidechain	95/166~(57%)	63/101~(62%)	32/47~(68%)	0/18~(0%)
Aromatic	0/12~(0%)	0/6~(0%)	0/5~(0%)	0/1~(0%)
Overall	153/256~(60%)	91/138~(66%)	47/84~(56%)	15/34~(44%)

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.

Random coil index (RCI) for chain A:

