



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:17 pm BST

PDB ID : 2LTS
Title : Solution structure of RDE-4(150-235)
Authors : Deshmukh, M.; Chiliveri, S.
Deposited on : 2012-05-31

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

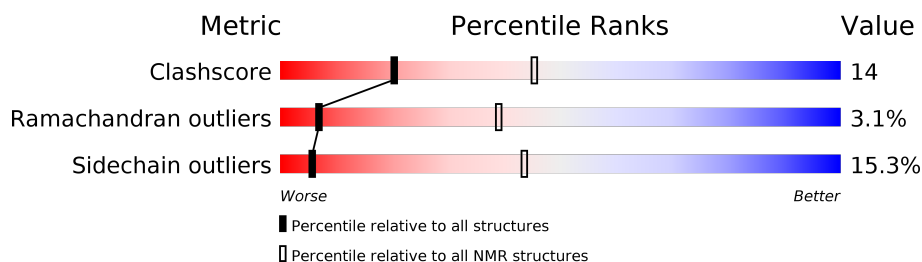
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	246	

2 Ensemble composition and analysis

This entry contains 10 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: *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:154-A:158, A:169-A:233 (70)	0.22	3

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 and 4 single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 8, 9, 10
Single-model clusters	1; 5; 6; 7

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1376 atoms, of which 690 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein RDE-4.

Mol	Chain	Residues	Atoms						Trace
1	A	86	Total	C	H	N	O	S	0
			1376	429	690	121	132	4	

There are 3 discrepancies between the modelled and reference sequences:

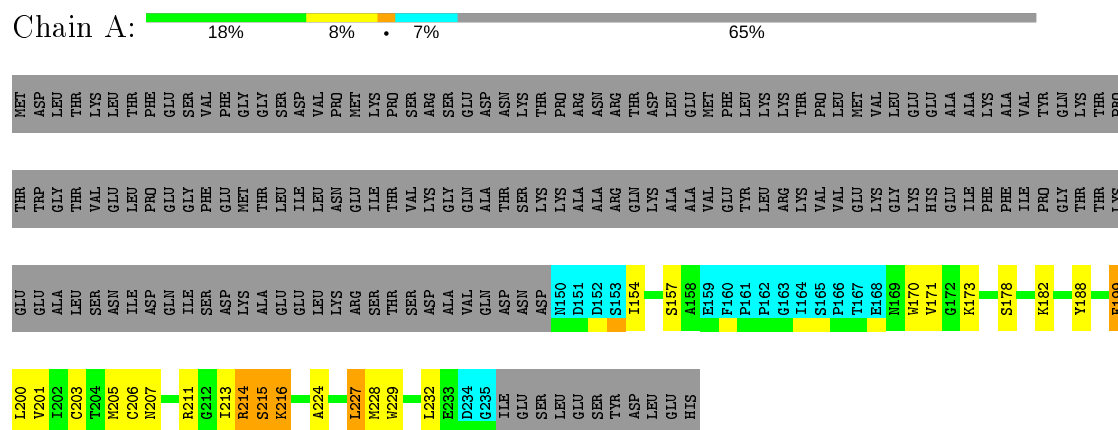
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	LEU	-	EXPRESSION TAG	UNP G5EBF5
A	245	GLU	-	EXPRESSION TAG	UNP G5EBF5
A	246	HIS	-	EXPRESSION TAG	UNP G5EBF5

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Protein RDE-4

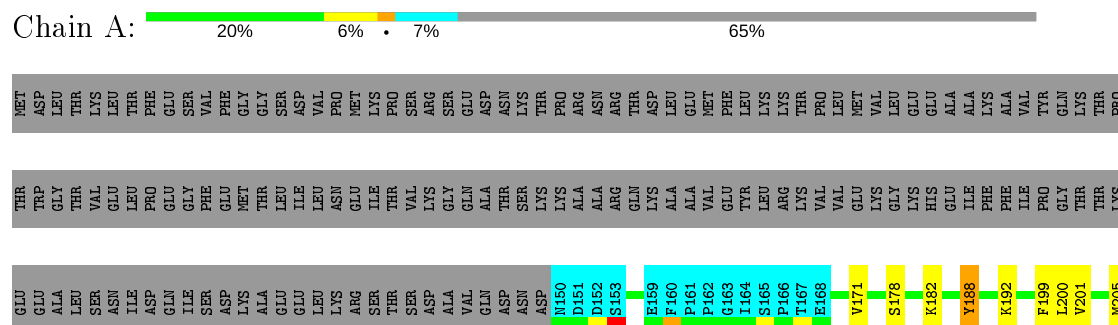


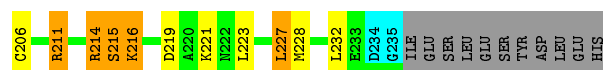
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

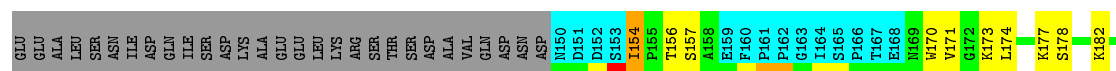
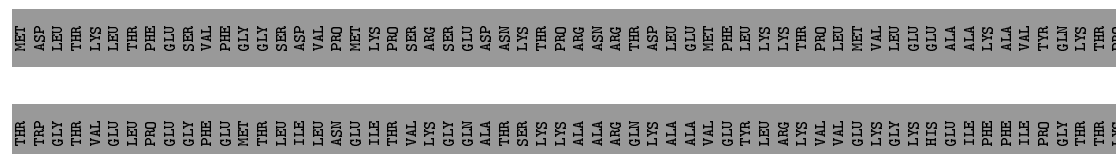
- Molecule 1: Protein RDE-4





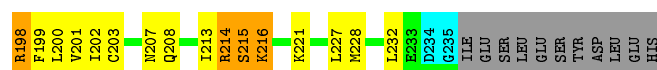
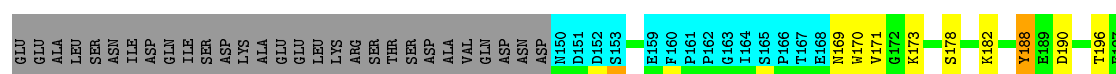
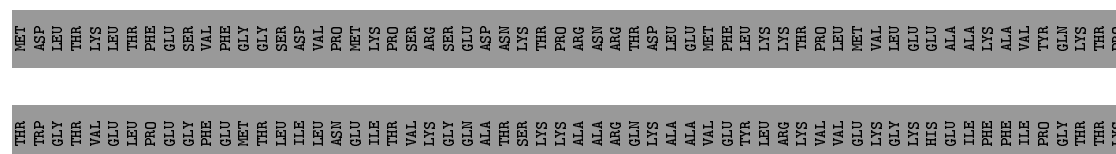
4.2.2 Score per residue for model 2

- Molecule 1: Protein RDE-4



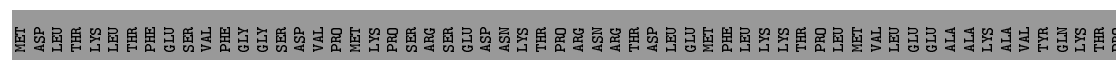
4.2.3 Score per residue for model 3 (medoid)

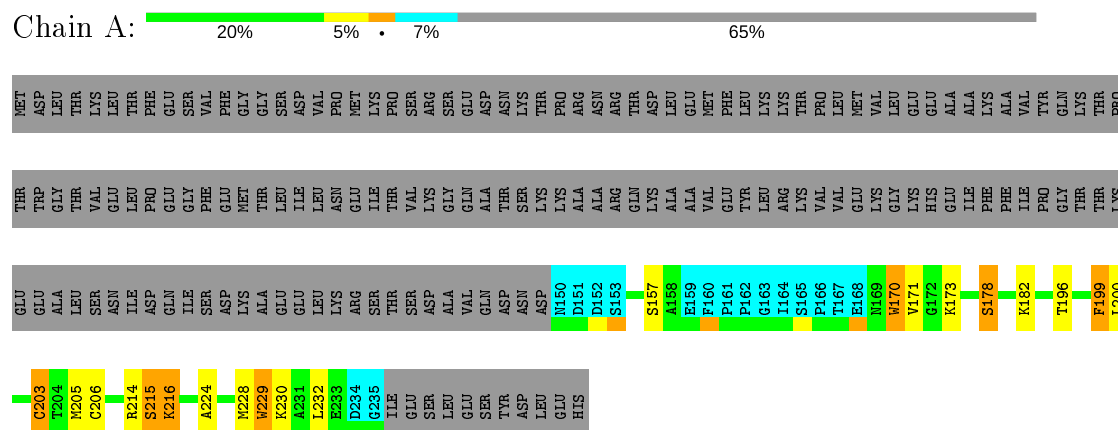
- Molecule 1: Protein RDE-4



4.2.4 Score per residue for model 4

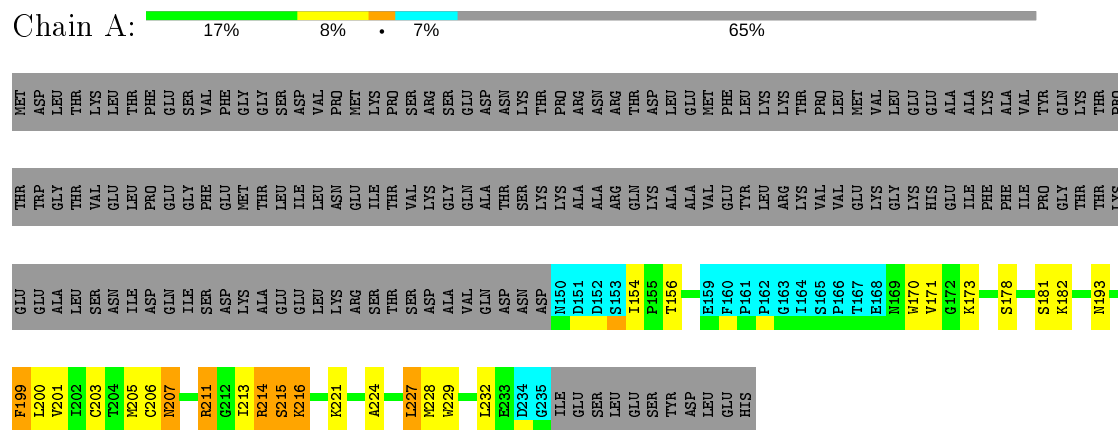
- Molecule 1: Protein RDE-4





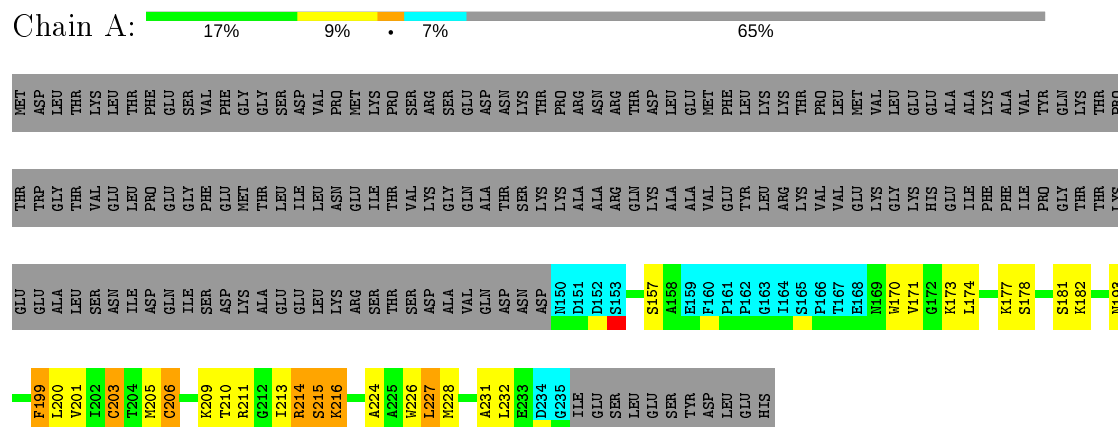
4.2.8 Score per residue for model 8

- Molecule 1: Protein RDE-4



4.2.9 Score per residue for model 9

- Molecule 1: Protein RDE-4



- Molecule 1: Protein RDE-4

D190	D191	D192	R198	F199	L200	V201	L202	C203	L204	M205	C206	N207	R211	R214	S215	K216	N222	L227	M228	L232	P233	D234	G235	I1E	G1U	SER	SER	LEU	GLU	SER	SER	GLU	ASP	ASP	M160	D151	D152	S163	I154	S167	A158	E159	F160	P161	P162	G163	I164	S165	T167	E168	M169	V171	G172	K173	L174	K177	K182	I183	G184
GLU	GLU	ALA	LEU	SER	ASN	ASP	ILE	SER	ASP	LYS	ALA	GLU	GLU	LEU	LYS	ARG	SER	THR	THR	ASP	ASN	ASP	M160	D151	D152	S163	I154	S167	A158	E159	F160	P161	P162	G163	I164	S165	T167	E168	M169	V171	G172	K173	L174	K177	K182	I183	G184												
THR	THR	GLY	THR	VAL	GLU	LEU	THR	PHE	GLU	GLU	THR	ILE	ILE	LEU	ASN	GLU	LYS	VAL	GLY	THR	SER	LYS	LYS	ALA	ALA	ARG	GLN	LYS	ALA	VAL	GLU	TYR	LEU	LEU	ARG	LYS	VAL	GLU	LYS	GLY	LYS	HIS	GLU	ILE	PHE	ALA	VAL	GLY	THR	THR									
MET	ASP	LEU	THR	LYS	LEU	PHE	GLU	VAL	PHE	GLY	GLY	SER	ASP	VAL	PRO	MET	LYS	ARG	SER	ASN	LYS	THR	PRO	ASN	GLU	ASP	THR	SER	LYS	THR	PRO	ASN	ARG	ARG	THR	ASP	LEU	GLU	MET	PHE	LEU	LYS	LYS	THR	PRO	LEU	GLU	ALA	ALA	LYS	ALA	VAL	GLN	LYS	THR	PRO			

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1435
Number of shifts mapped to atoms	1435
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	569	596	596	16±4
All	All	5690	5960	5960	159

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:CYS:SG	1:A:224:ALA:HB1	0.75	2.21	7	5
1:A:213:ILE:N	1:A:213:ILE:HD12	0.63	2.07	3	1
1:A:158:ALA:HB1	1:A:214:ARG:HH12	0.62	1.54	6	1
1:A:226:TRP:CZ3	1:A:229:TRP:CD1	0.62	2.88	6	1
1:A:229:TRP:CD1	1:A:230:LYS:N	0.61	2.69	6	2
1:A:188:TYR:CD1	1:A:188:TYR:N	0.60	2.68	5	3
1:A:200:LEU:HD12	1:A:200:LEU:C	0.60	2.17	9	6
1:A:154:ILE:O	1:A:156:THR:HG23	0.59	1.96	2	1
1:A:200:LEU:C	1:A:200:LEU:HD12	0.59	2.17	4	4
1:A:226:TRP:CH2	1:A:229:TRP:NE1	0.59	2.71	6	1
1:A:158:ALA:HB1	1:A:214:ARG:NH1	0.58	2.14	6	1
1:A:178:SER:O	1:A:182:LYS:N	0.58	2.37	2	10
1:A:199:PHE:N	1:A:199:PHE:CD1	0.55	2.74	6	1
1:A:213:ILE:N	1:A:213:ILE:HD13	0.54	2.16	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:TRP:O	1:A:173:LYS:N	0.54	2.40	2	8
1:A:206:CYS:SG	1:A:207:ASN:N	0.54	2.80	10	1
1:A:213:ILE:CD1	1:A:213:ILE:N	0.54	2.70	3	1
1:A:190:ASP:OD1	1:A:201:VAL:HG22	0.53	2.03	10	1
1:A:215:SER:O	1:A:216:LYS:O	0.52	2.28	9	10
1:A:170:TRP:CE3	1:A:222:ASN:OD1	0.52	2.63	10	1
1:A:228:MET:O	1:A:232:LEU:N	0.51	2.43	7	10
1:A:203:CYS:SG	1:A:224:ALA:O	0.50	2.69	7	1
1:A:205:MET:O	1:A:207:ASN:N	0.50	2.44	8	2
1:A:226:TRP:O	1:A:226:TRP:CD1	0.50	2.65	9	1
1:A:174:LEU:O	1:A:177:LYS:N	0.50	2.44	9	3
1:A:213:ILE:HD13	1:A:213:ILE:N	0.50	2.22	5	2
1:A:226:TRP:CZ3	1:A:229:TRP:NE1	0.48	2.81	6	1
1:A:184:GLN:NE2	1:A:206:CYS:SG	0.48	2.87	4	1
1:A:199:PHE:O	1:A:214:ARG:O	0.48	2.32	5	10
1:A:211:ARG:O	1:A:227:LEU:CD1	0.47	2.63	1	7
1:A:203:CYS:SG	1:A:224:ALA:CB	0.47	2.99	7	2
1:A:200:LEU:HD12	1:A:201:VAL:N	0.47	2.24	3	5
1:A:158:ALA:CB	1:A:214:ARG:HH12	0.47	2.20	6	1
1:A:203:CYS:SG	1:A:228:MET:SD	0.46	3.04	3	1
1:A:173:LYS:O	1:A:177:LYS:CG	0.46	2.63	4	1
1:A:211:ARG:CD	1:A:211:ARG:C	0.46	2.83	8	1
1:A:170:TRP:NE1	1:A:226:TRP:CE3	0.46	2.84	6	1
1:A:215:SER:OG	1:A:216:LYS:N	0.45	2.48	8	3
1:A:201:VAL:HG21	1:A:221:LYS:HG2	0.45	1.88	8	3
1:A:199:PHE:CD1	1:A:199:PHE:N	0.45	2.84	3	1
1:A:205:MET:O	1:A:206:CYS:C	0.44	2.56	5	6
1:A:170:TRP:CZ3	1:A:222:ASN:OD1	0.44	2.70	10	1
1:A:188:TYR:N	1:A:188:TYR:CD1	0.44	2.85	3	1
1:A:190:ASP:OD1	1:A:190:ASP:O	0.44	2.36	5	1
1:A:214:ARG:O	1:A:215:SER:O	0.44	2.36	3	1
1:A:206:CYS:O	1:A:207:ASN:OD1	0.44	2.36	6	1
1:A:200:LEU:C	1:A:200:LEU:CD1	0.44	2.86	1	3
1:A:215:SER:OG	1:A:219:ASP:OD2	0.44	2.36	5	2
1:A:223:LEU:O	1:A:227:LEU:N	0.43	2.51	1	1
1:A:190:ASP:OD1	1:A:190:ASP:N	0.43	2.51	3	1
1:A:200:LEU:CD1	1:A:200:LEU:C	0.43	2.84	5	6
1:A:194:GLU:O	1:A:197:GLU:OE2	0.43	2.36	4	1
1:A:201:VAL:HG21	1:A:221:LYS:CG	0.43	2.44	8	4
1:A:213:ILE:N	1:A:213:ILE:CD1	0.43	2.79	6	1
1:A:206:CYS:O	1:A:207:ASN:ND2	0.43	2.51	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:ASP:O	1:A:190:ASP:OD1	0.42	2.38	4	1
1:A:211:ARG:NE	1:A:213:ILE:HD11	0.42	2.29	8	1
1:A:229:TRP:CD1	1:A:229:TRP:C	0.42	2.89	6	1
1:A:207:ASN:O	1:A:208:GLN:NE2	0.41	2.53	3	1
1:A:198:ARG:CG	1:A:199:PHE:H	0.41	2.29	3	1
1:A:158:ALA:CA	1:A:214:ARG:HH12	0.41	2.29	6	1
1:A:229:TRP:CZ2	1:A:233:GLU:OE2	0.41	2.74	6	1
1:A:214:ARG:NH1	1:A:214:ARG:CG	0.40	2.83	3	1
1:A:174:LEU:HD21	1:A:228:MET:HB3	0.40	1.93	4	1
1:A:214:ARG:CG	1:A:214:ARG:HH11	0.40	2.30	3	1
1:A:192:LYS:CB	1:A:198:ARG:O	0.40	2.69	10	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	70/246 (28%)	62±1 (89±2%)	6±1 (8±2%)	2±0 (3±1%)	7	39
All	All	700/2460 (28%)	623 (89%)	55 (8%)	22 (3%)	7	39

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	216	LYS	10
1	A	215	SER	10
1	A	206	CYS	2

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/218 (28%)	53±3 (85±4%)	10±3 (15±4%)	6	43
All	All	620/2180 (28%)	525 (85%)	95 (15%)	6	43

All 32 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	171	VAL	10
1	A	227	LEU	9
1	A	199	PHE	7
1	A	214	ARG	7
1	A	203	CYS	6
1	A	157	SER	6
1	A	188	TYR	5
1	A	154	ILE	4
1	A	206	CYS	4
1	A	170	TRP	3
1	A	196	THR	3
1	A	229	TRP	3
1	A	178	SER	3
1	A	232	LEU	2
1	A	181	SER	2
1	A	210	THR	2
1	A	207	ASN	2
1	A	193	ASN	2
1	A	211	ARG	2
1	A	209	LYS	1
1	A	198	ARG	1
1	A	187	ILE	1
1	A	192	LYS	1
1	A	184	GLN	1
1	A	205	MET	1
1	A	202	ILE	1
1	A	204	THR	1
1	A	213	ILE	1
1	A	173	LYS	1
1	A	169	ASN	1
1	A	156	THR	1
1	A	222	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [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 41% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	1435
Number of shifts mapped to atoms	1435
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	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	242	0.59 ± 0.24	Should be applied
$^{13}\text{C}_\beta$	227	1.31 ± 0.20	Should be applied
$^{13}\text{C}'$	241	0.12 ± 0.18	None needed (< 0.5 ppm)
^{15}N	225	-0.47 ± 0.39	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 41%, i.e. 376 atoms were assigned a chemical shift out of a possible 925. 7 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	267/346 (77%)	65/138 (47%)	137/140 (98%)	65/68 (96%)
Sidechain	106/526 (20%)	21/312 (7%)	85/183 (46%)	0/31 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	3/53 (6%)	2/27 (7%)	0/23 (0%)	1/3 (33%)
Overall	376/925 (41%)	88/477 (18%)	222/346 (64%)	66/102 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 447 atoms were assigned a chemical shift out of a possible 1090. 7 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	323/420 (77%)	78/167 (47%)	167/172 (97%)	78/81 (96%)
Sidechain	121/608 (20%)	22/361 (6%)	99/215 (46%)	0/32 (0%)
Aromatic	3/62 (5%)	2/32 (6%)	0/27 (0%)	1/3 (33%)
Overall	447/1090 (41%)	102/560 (18%)	266/414 (64%)	79/116 (68%)

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:

