



Full wwPDB NMR Structure Validation Report ⓘ

Sep 7, 2020 – 02:34 PM BST

PDB ID : 6RWG
Title : Structure of HIV-1 CAcSP1NC mutant(W41A,M42A) interacting with maturation inhibitor EP39
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Deposited on : 2019-06-05

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 : 2.14.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.2

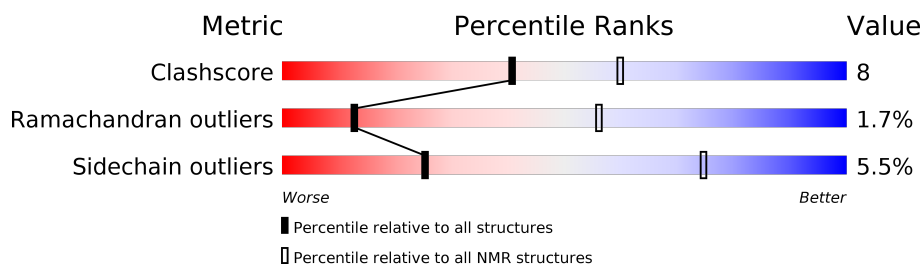
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 45%.

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	157	<div>32% 8% • 59%</div>

2 Ensemble composition and analysis

This entry contains 10 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:9-A:62, A:68-A:78 (65)	0.83	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2435 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gag polypeptide.

Mol	Chain	Residues	Atoms						Trace
1	A	157	Total	C	H	N	O	S	0
			2433	744	1221	229	225	14	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	TRP	engineered mutation	UNP E7DAY8
A	42	ALA	MET	engineered mutation	UNP E7DAY8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

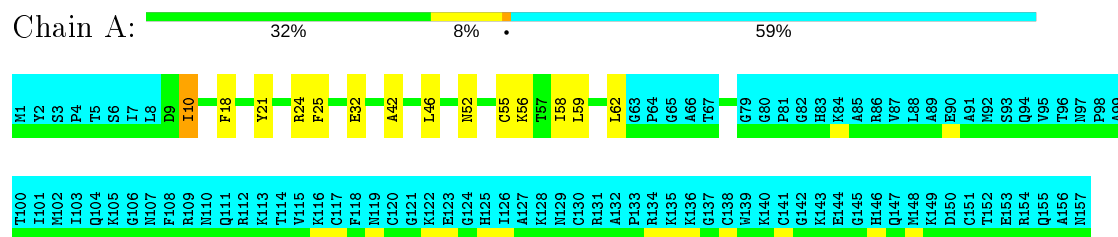
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

4 Residue-property plots

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: Gag polypeptide

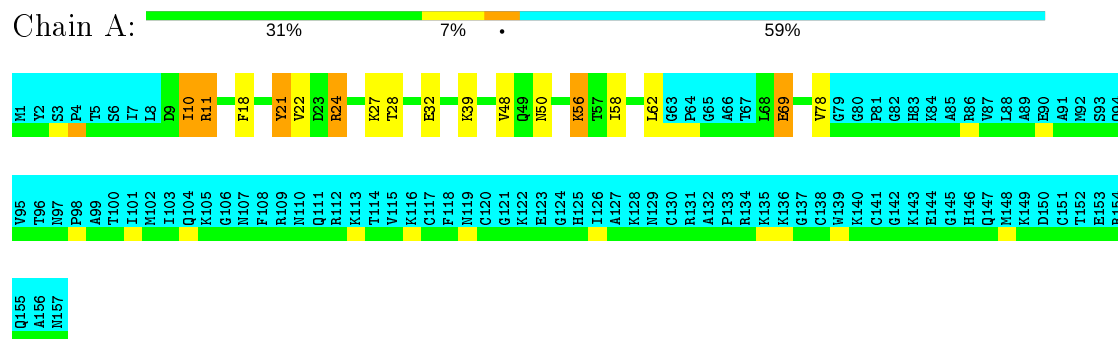


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

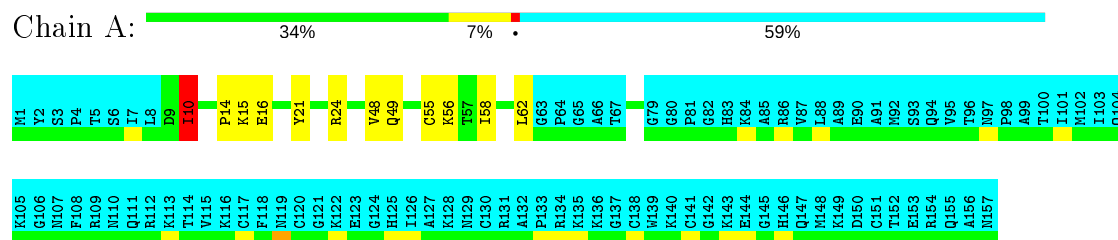
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Gag polypeptide



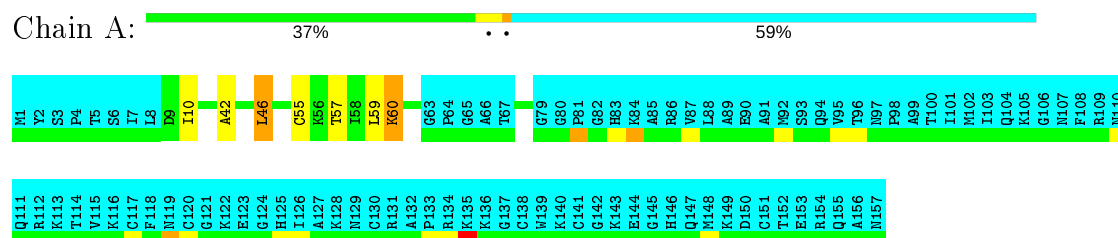
4.2.2 Score per residue for model 2

- Molecule 1: Gag polypeptide



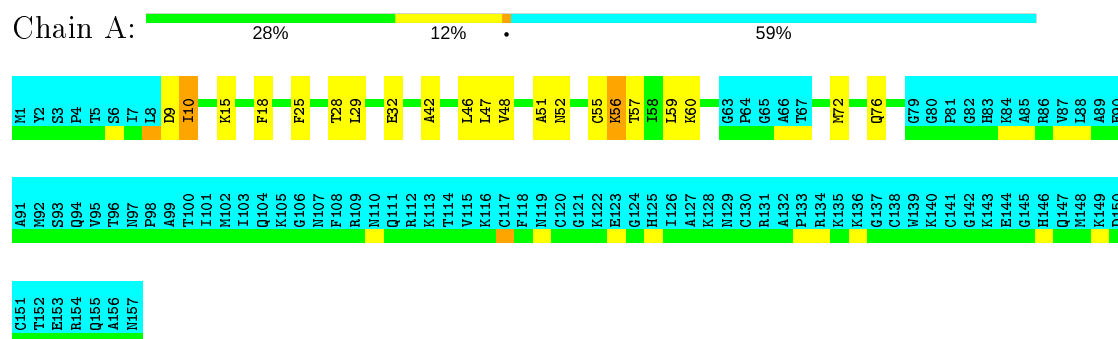
4.2.3 Score per residue for model 3

- Molecule 1: Gag polypeptide



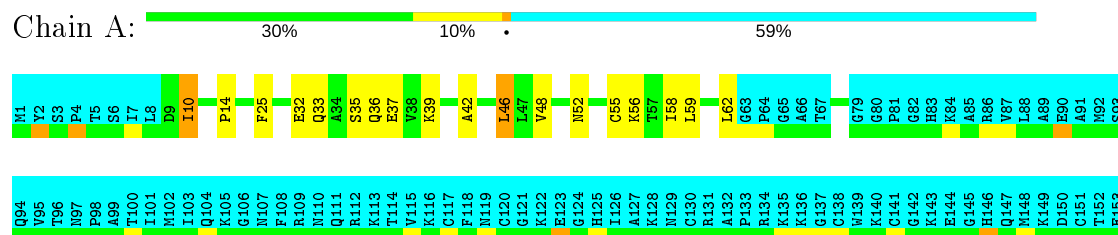
4.2.4 Score per residue for model 4

- Molecule 1: Gag polypeptide



4.2.5 Score per residue for model 5

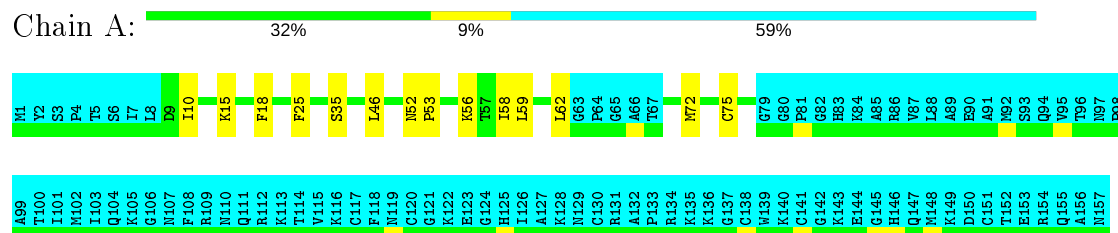
- Molecule 1: Gag polypeptide



R154
Q155
A156
N157

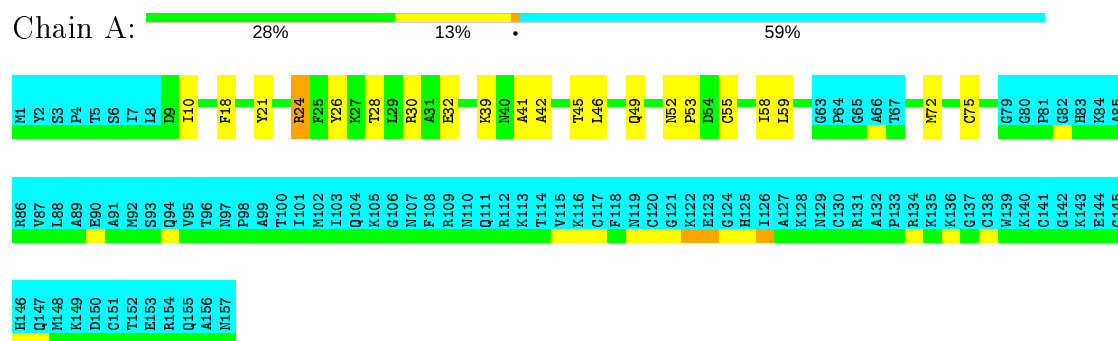
4.2.6 Score per residue for model 6

- Molecule 1: Gag polyprotein



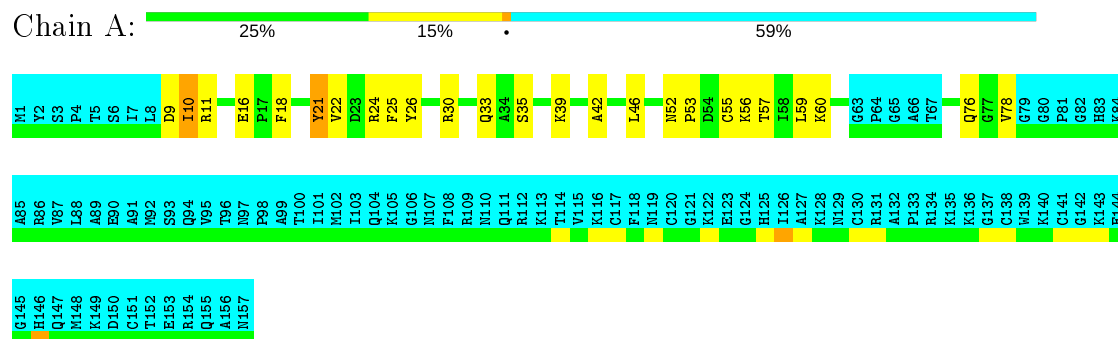
4.2.7 Score per residue for model 7

- Molecule 1: Gag polyprotein



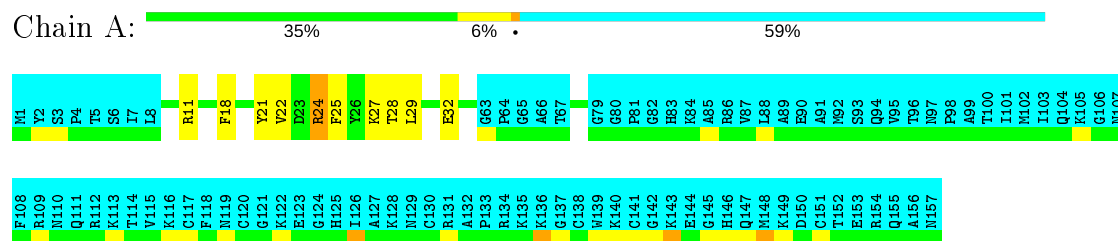
4.2.8 Score per residue for model 8

- Molecule 1: Gag polyprotein



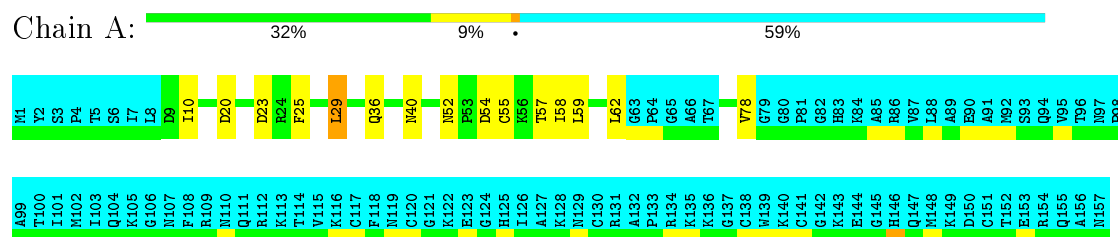
4.2.9 Score per residue for model 9

- Molecule 1: Gag polyprotein



4.2.10 Score per residue for model 10

- Molecule 1: Gag polyprotein



5 Refinement protocol and experimental data overview

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

Of the 500 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
ARIA	structure calculation	2.3.2
CNS	refinement	1.2

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	1074
Number of shifts mapped to atoms	922
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	152
Assignment completeness (well-defined parts)	45%

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

6 Model quality

6.1 Standard geometry

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

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	515	517	517	8±3
All	All	5170	5170	5170	78

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ALA:HB3	1:A:56:LYS:HD3	0.86	1.45	4	1
1:A:35:SER:O	1:A:39:LYS:HG2	0.65	1.92	5	1
1:A:42:ALA:O	1:A:46:LEU:HB2	0.61	1.95	3	3
1:A:58:ILE:O	1:A:62:LEU:HG	0.61	1.95	1	5
1:A:48:VAL:O	1:A:56:LYS:HG2	0.60	1.97	2	2
1:A:18:PHE:CD1	1:A:72:MET:HA	0.60	2.31	4	3
1:A:52:ASN:HB3	1:A:55:CYS:SG	0.59	2.37	7	5
1:A:59:LEU:HD21	1:A:75:CYS:SG	0.59	2.37	6	1
1:A:42:ALA:O	1:A:46:LEU:HB3	0.58	1.98	7	2
1:A:25:PHE:O	1:A:29:LEU:HG	0.58	1.97	4	2
1:A:24:ARG:O	1:A:27:LYS:HG2	0.58	1.99	1	2
1:A:35:SER:O	1:A:39:LYS:HG3	0.54	2.01	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:THR:O	1:A:32:GLU:HG2	0.54	2.01	1	4
1:A:16:GLU:HG2	1:A:21:TYR:CD1	0.53	2.38	8	1
1:A:14:PRO:HA	1:A:55:CYS:SG	0.53	2.43	2	1
1:A:55:CYS:O	1:A:59:LEU:HG	0.52	2.04	10	6
1:A:30:ARG:O	1:A:33:GLN:HG2	0.51	2.04	8	1
1:A:54:ASP:O	1:A:57:THR:HB	0.51	2.06	10	1
1:A:18:PHE:HA	1:A:21:TYR:CE1	0.51	2.41	9	1
1:A:72:MET:O	1:A:76:GLN:HG3	0.51	2.06	4	1
1:A:9:ASP:O	1:A:11:ARG:HG3	0.50	2.06	8	1
1:A:57:THR:O	1:A:60:LYS:HG2	0.49	2.08	4	3
1:A:48:VAL:O	1:A:56:LYS:HD2	0.49	2.06	5	1
1:A:10:ILE:HD13	1:A:25:PHE:CD1	0.49	2.43	6	1
1:A:59:LEU:HD11	1:A:75:CYS:SG	0.48	2.49	7	1
1:A:11:ARG:HD2	1:A:11:ARG:O	0.48	2.09	8	2
1:A:21:TYR:O	1:A:24:ARG:HG3	0.47	2.10	9	1
1:A:20:ASP:O	1:A:23:ASP:HB3	0.47	2.09	10	1
1:A:51:ALA:HB3	1:A:56:LYS:CD	0.46	2.32	4	1
1:A:48:VAL:O	1:A:56:LYS:HE2	0.46	2.11	1	1
1:A:21:TYR:HA	1:A:24:ARG:CZ	0.45	2.41	7	1
1:A:11:ARG:HA	1:A:50:ASN:ND2	0.45	2.26	1	1
1:A:25:PHE:O	1:A:29:LEU:HB2	0.45	2.12	10	1
1:A:52:ASN:OD1	1:A:53:PRO:HD2	0.43	2.13	7	3
1:A:21:TYR:CD2	1:A:24:ARG:HD3	0.43	2.49	1	1
1:A:26:TYR:O	1:A:30:ARG:HG3	0.43	2.13	7	1
1:A:47:LEU:HD13	1:A:47:LEU:O	0.42	2.14	4	1
1:A:36:GLN:HG2	1:A:37:GLU:N	0.42	2.29	5	1
1:A:55:CYS:O	1:A:58:ILE:HG13	0.42	2.13	7	1
1:A:49:GLN:HA	1:A:56:LYS:NZ	0.42	2.29	2	1
1:A:26:TYR:O	1:A:30:ARG:HG2	0.42	2.14	8	1
1:A:69:GLU:CD	1:A:69:GLU:H	0.42	2.18	1	1
1:A:41:ALA:O	1:A:45:THR:HG22	0.41	2.16	7	1
1:A:36:GLN:HB3	1:A:40:ASN:ND2	0.41	2.31	10	1
1:A:18:PHE:H	1:A:76:GLN:HB3	0.41	1.75	8	1
1:A:18:PHE:O	1:A:22:VAL:HG23	0.41	2.15	8	3
1:A:32:GLU:O	1:A:39:LYS:HE2	0.40	2.17	1	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	65/157 (41%)	59±1 (91±2%)	5±1 (7±2%)	1±1 (2±1%)	13	56
All	All	650/1570 (41%)	594 (91%)	45 (7%)	11 (2%)	13	56

All 4 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	10	ILE	6
1	A	78	VAL	3
1	A	35	SER	1
1	A	14	PRO	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	56/129 (43%)	53±2 (94±3%)	3±2 (6±3%)	25	74
All	All	560/1290 (43%)	529 (94%)	31 (6%)	25	74

All 14 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	10	ILE	5
1	A	24	ARG	5
1	A	56	LYS	4
1	A	21	TYR	3
1	A	46	LEU	3
1	A	15	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	69	GLU	1
1	A	16	GLU	1
1	A	25	PHE	1
1	A	60	LYS	1
1	A	11	ARG	1
1	A	39	LYS	1
1	A	29	LEU	1
1	A	49	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 45% for the well-defined parts and 40% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1074
Number of shifts mapped to atoms	922
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	152
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atoms found in structure. All 152 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	79	GLY	HN	8.56	0.002	1
A	137	GLY	HN	8.109	0.001	1
A	63	GLY	HN	7.502	0.002	1
A	136	LYS	HN	8.395	0.003	1
A	87	VAL	HN	8.089	0.001	1
A	114	THR	HN	8.142	0.002	1
A	123	GLU	HN	8.354	0.002	1
A	31	ALA	HN	7.548	0.002	1
A	133	PRO	HG1	1.98	-1.0	1
A	122	LYS	HD1	1.585	-1.0	1
A	139	TRP	HN	8.379	0.007	1
A	71	MET	HN	8.401	0.002	1
A	52	ASN	HN	8.986	0.002	1
A	149	LYS	HN	8.476	0.005	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	126	ILE	HN	7.797	0.004	1
A	39	LYS	HN	8.28	0.004	1
A	135	LYS	HN	8.568	0.004	1
A	51	ALA	HN	7.28	0.004	1
A	132	ALA	HN	8.703	0.001	1
A	45	THR	HN	7.727	0.003	1
A	89	ALA	HN	8.152	0.001	1
A	8	LEU	HN	7.546	0.002	1
A	47	LEU	HN	7.562	0.001	1
A	133	PRO	HD1	3.51	0.0	1
A	49	GLN	HN	7.872	0.002	1
A	68	LEU	HN	8.862	0.004	1
A	146	HIS	HN	7.121	0.001	1
A	82	GLY	HN	8.511	0.001	1
A	134	ARG	HN	8.351	0.004	1
A	75	CYS	HN	7.572	0.002	1
A	118	PHE	HN	8.54	0.003	1
A	107	ASN	HN	8.185	0.0	1
A	35	SER	HN	8.11	0.002	1
A	108	PHE	HN	8.126	0.001	1
A	54	ASP	HN	7.922	0.003	1
A	21	TYR	HN	7.553	0.004	1
A	92	MET	HN	8.164	0.001	1
A	4	PRO	HG1	1.928	0.0	1
A	140	LYS	HN	9.341	0.003	1
A	44	GLU	HN	8.475	0.008	1
A	5	THR	HN	8.125	0.004	1
A	56	LYS	HN	9.247	0.002	1
A	74	ALA	HN	7.878	0.004	1
A	69	GLU	HN	8.575	0.002	1
A	120	CYS	HN	8.856	0.002	1
A	33	GLN	HN	8.139	0.002	1
A	148	MET	HN	8.833	0.001	1
A	24	ARG	HN	7.921	0.002	1
A	144	GLU	HN	8.214	0.001	1
A	154	ARG	HN	8.355	0.003	1
A	7	ILE	HN	8.346	0.003	1
A	127	ALA	HN	8.71	0.003	1
A	73	THR	HN	8.022	0.003	1
A	88	LEU	HN	8.213	0.001	1
A	62	LEU	HN	7.46	0.002	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	94	GLN	HN	8.253	0.002	1
A	48	VAL	HN	7.488	0.002	1
A	100	THR	HN	7.884	0.008	1
A	16	GLU	HN	7.066	0.003	1
A	40	ASN	HN	8.423	0.007	1
A	37	GLU	HN	8.449	0.003	1
A	84	LYS	HN	8.386	0.001	1
A	77	GLY	HN	8.334	0.006	1
A	138	CYS	HN	8.13	0.008	1
A	15	LYS	HN	8.511	0.001	1
A	143	LYS	HN	8.394	0.005	1
A	125	HIS	HN	7.15	0.001	1
A	150	ASP	HN	7.815	0.002	1
A	101	ILE	HN	7.842	0.001	1
A	78	VAL	HN	7.592	0.003	1
A	103	ILE	HN	7.992	0.0	1
A	41	ALA	HN	8.163	0.002	1
A	28	THR	HN	7.674	0.003	1
A	6	SER	HN	8.415	0.004	1
A	141	CYS	HN	8.476	0.006	1
A	46	LEU	HN	7.8	0.001	1
A	19	ARG	HN	9.138	0.001	1
A	23	ASP	HN	7.472	0.001	1
A	20	ASP	HN	6.981	0.003	1
A	30	ARG	HN	7.953	0.003	1
A	50	ASN	HN	7.778	0.005	1
A	152	THR	HN	8.115	0.002	1
A	34	ALA	HN	7.959	0.002	1
A	122	LYS	HN	8.086	0.006	1
A	10	ILE	HN	7.436	0.004	1
A	155	GLN	HN	8.405	0.0	1
A	72	MET	HN	8.616	0.005	1
A	106	GLY	HN	8.288	0.001	1
A	4	PRO	HD1	3.612	0.0	1
A	18	PHE	HN	9.202	0.001	1
A	59	LEU	HN	8.597	0.002	1
A	121	GLY	HN	7.853	0.005	1
A	95	VAL	HN	8.033	0.006	1
A	29	LEU	HN	7.898	0.004	1
A	91	ALA	HN	8.139	0.001	1
A	61	ALA	HN	7.186	0.006	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	67	THR	HN	8.56	0.002	1
A	147	GLN	HN	8.873	0.007	1
A	119	ASN	HN	9.523	0.009	1
A	25	PHE	HN	8.955	0.002	1
A	55	CYS	HN	8.287	0.002	1
A	13	GLY	HN	9.844	0.002	1
A	42	ALA	HN	8.281	0.005	1
A	115	VAL	HN	8.345	0.002	1
A	22	VAL	HN	8.245	0.004	1
A	157	ASN	HN	7.941	0.001	1
A	66	ALA	HN	7.154	0.002	1
A	116	LYS	HN	8.092	0.004	1
A	104	GLN	HN	8.318	0.003	1
A	151	CYS	HN	7.547	0.001	1
A	85	ALA	HN	8.225	0.002	1
A	9	ASP	HN	7.651	0.002	1
A	32	GLU	HN	7.871	0.001	1
A	145	GLY	HN	8.522	0.005	1
A	102	MET	HN	8.208	0.002	1
A	76	GLN	HN	7.614	0.002	1
A	128	LYS	HN	8.19	0.001	1
A	129	ASN	HN	7.872	0.003	1
A	57	THR	HN	7.744	0.003	1
A	90	GLU	HN	8.265	0.002	1
A	97	ASN	HN	8.356	0.002	1
A	43	THR	HN	8.132	0.005	1
A	12	GLN	HN	7.615	0.002	1
A	58	ILE	HN	7.044	0.006	1
A	26	TYR	HN	8.614	0.003	1
A	4	PRO	HB1	2.222	0.0	1
A	131	ARG	HN	8.626	0.001	1
A	153	GLU	HN	8.601	0.003	1
A	38	VAL	HN	7.77	0.002	1
A	70	GLU	HN	7.714	0.001	1
A	86	ARG	HN	8.213	0.0	1
A	110	ASN	HN	8.245	0.001	1
A	27	LYS	HN	8.326	0.006	1
A	142	GLY	HN	8.112	0.002	1
A	65	GLY	HN	8.712	0.002	1
A	105	LYS	HN	8.289	0.001	1
A	39	LYS	HE1	2.918	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	80	GLY	HN	8.044	0.002	1
A	96	THR	HN	8.121	0.003	1
A	156	ALA	HN	8.331	0.001	1
A	130	CYS	HN	7.637	0.005	1
A	36	GLN	HN	8.492	0.001	1
A	11	ARG	HN	8.246	0.003	1
A	83	HIS	HN	8.203	0.004	1
A	116	LYS	HG1	0.992	0.001	1
A	117	CYS	HN	8.21	0.003	1
A	60	LYS	HN	8.322	0.005	1
A	99	ALA	HN	8.223	0.004	1
A	124	GLY	HN	8.603	0.003	1
A	93	SER	HN	8.114	0.001	1
A	109	ARG	HN	8.108	0.001	1
A	113	LYS	HN	8.151	0.001	1

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
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	144	-0.56 ± 0.28	None needed (imprecise)

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 45%, i.e. 362 atoms were assigned a chemical shift out of a possible 813. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	127/319 (40%)	65/127 (51%)	0/130 (0%)	62/62 (100%)
Sidechain	219/460 (48%)	214/269 (80%)	0/166 (0%)	5/25 (20%)
Aromatic	16/34 (47%)	16/18 (89%)	0/16 (0%)	0/0 (—%)
Overall	362/813 (45%)	295/414 (71%)	0/312 (0%)	67/87 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 767 atoms were assigned a chemical shift out of a possible

1935. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	297/769 (39%)	153/306 (50%)	0/314 (0%)	144/149 (97%)
Sidechain	444/1072 (41%)	436/636 (69%)	0/371 (0%)	8/65 (12%)
Aromatic	26/94 (28%)	25/50 (50%)	0/39 (0%)	1/5 (20%)
Overall	767/1935 (40%)	614/992 (62%)	0/724 (0%)	153/219 (70%)

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:

