



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:59 AM UTC

PDB ID : 5M1G / pdb_00005m1g
BMRB ID : 34049
Title : Structure of a Spumaretrovirus Gag central domain reveals an ancient retro-viral capsid
Authors : Nicastro, G.; Ball, N.; Taylor, I.A.
Deposited on : 2016-10-07

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

MolProbity : 4-5-2 with Phenix2.0
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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

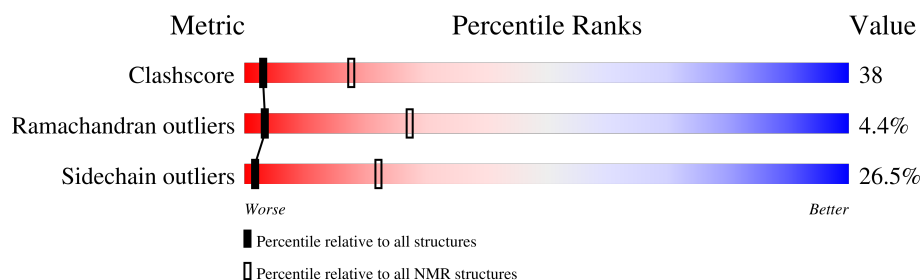
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

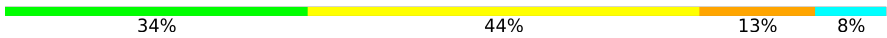
The overall completeness of chemical shifts assignment is 41%.

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	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	99	
1	B	99	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:386-A:476, B:386-B:476 (182)	0.32	8

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3086 atoms, of which 1548 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gag protein.

Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1543	480	774	139	147	3	
1	B	99	Total	C	H	N	O	S	0
			1543	480	774	139	147	3	

There are 6 discrepancies between the modelled and reference sequences:

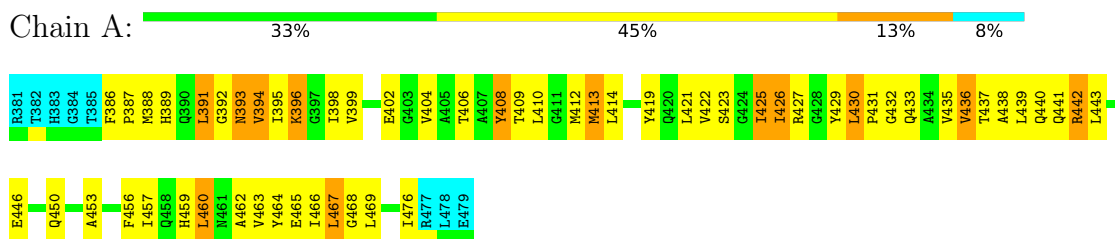
Chain	Residue	Modelled	Actual	Comment	Reference
A	449	ASP	ASN	conflict	UNP P14349
A	478	LEU	-	expression tag	UNP P14349
A	479	GLU	-	expression tag	UNP P14349
B	449	ASP	ASN	conflict	UNP P14349
B	478	LEU	-	expression tag	UNP P14349
B	479	GLU	-	expression tag	UNP P14349

4 Residue-property plots

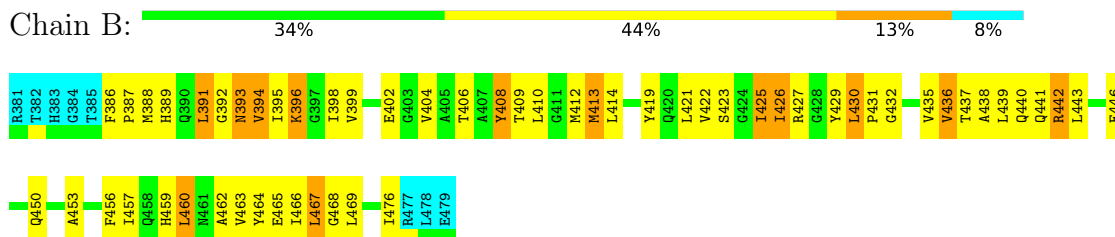
4.1 Average score per residue in the NMR ensemble

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 protein



- Molecule 1: Gag protein

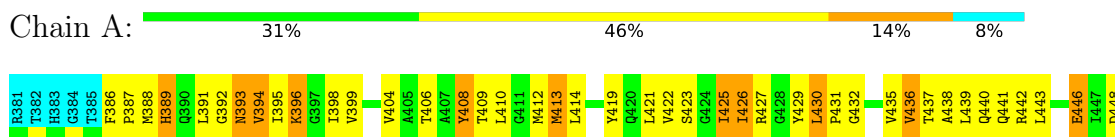


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

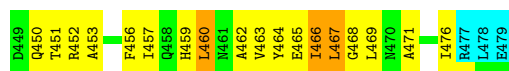
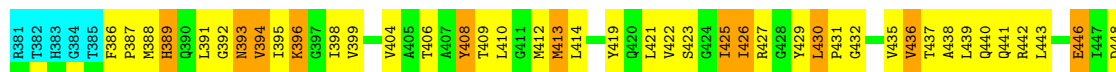
- Molecule 1: Gag protein





• Molecule 1: Gag protein

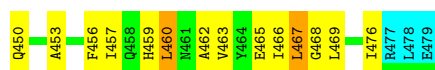
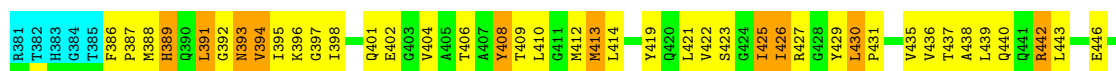
Chain B: 31% 46% 14% 8%



4.2.2 Score per residue for model 2

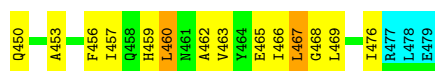
• Molecule 1: Gag protein

Chain A: 36% 43% 12% 8%



• Molecule 1: Gag protein

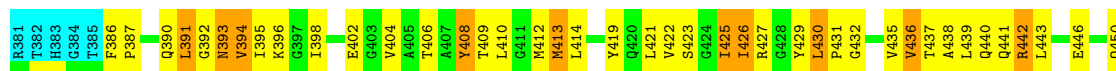
Chain B: 36% 44% 11% 8%



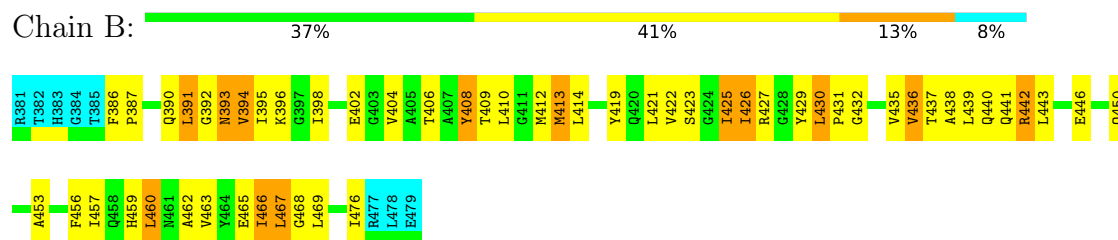
4.2.3 Score per residue for model 3

• Molecule 1: Gag protein

Chain A: 37% 41% 13% 8%

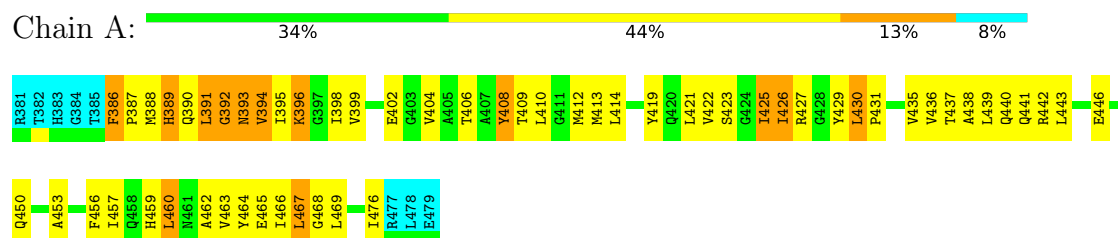


• Molecule 1: Gag protein

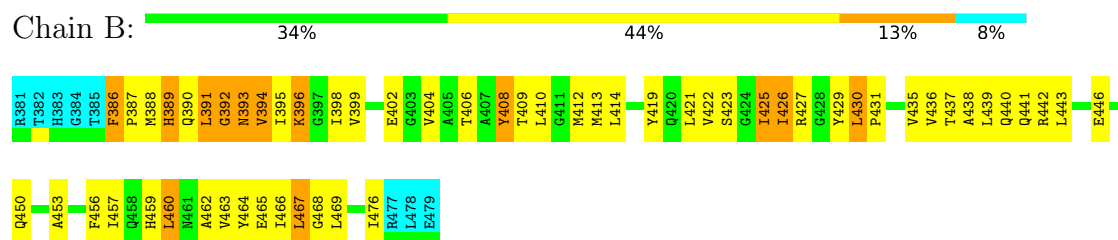


4.2.4 Score per residue for model 4

- Molecule 1: Gag protein

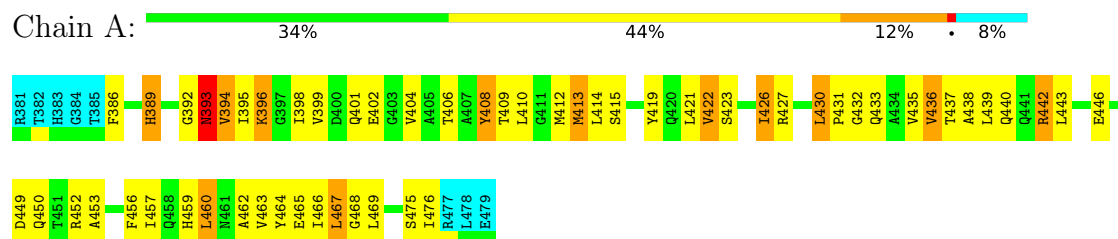


- Molecule 1: Gag protein

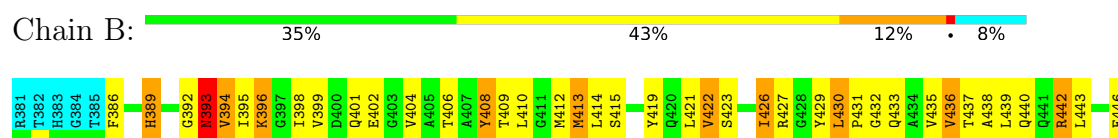


4.2.5 Score per residue for model 5

- Molecule 1: Gag protein



- Molecule 1: Gag protein



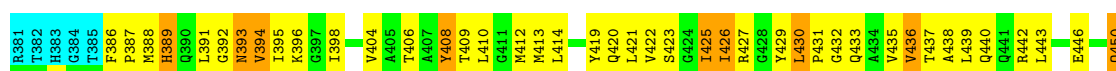


4.2.6 Score per residue for model 6

- Molecule 1: Gag protein



- Molecule 1: Gag protein

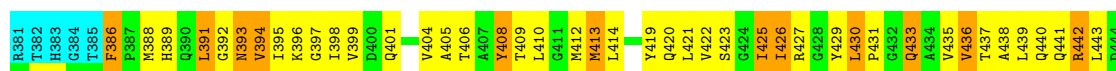


4.2.7 Score per residue for model 7

- Molecule 1: Gag protein

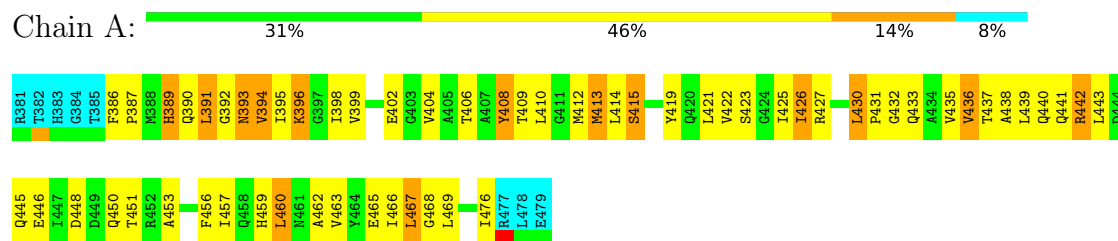


- Molecule 1: Gag protein

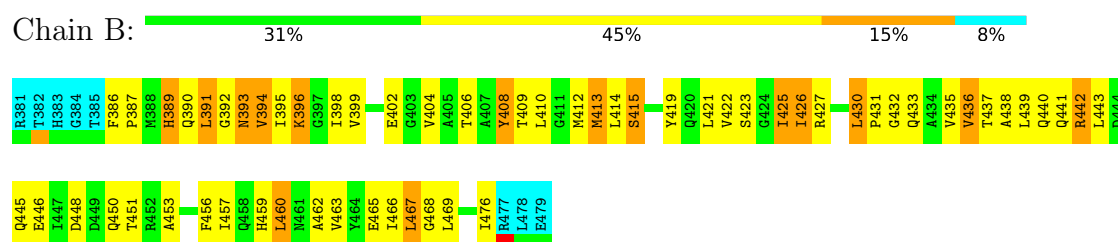


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Gag protein

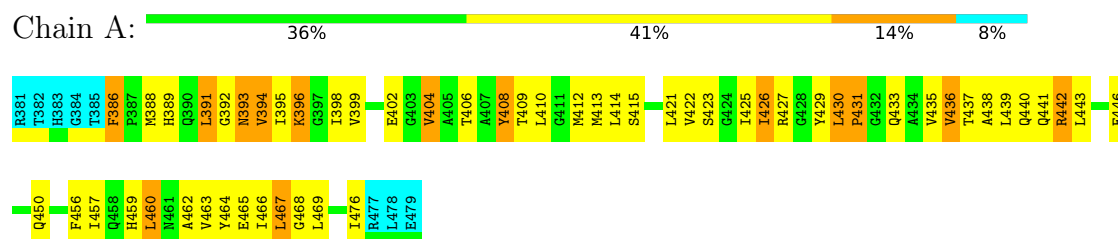


- Molecule 1: Gag protein

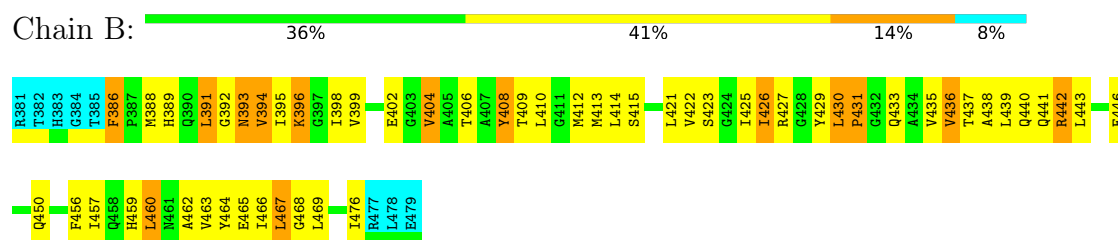


4.2.9 Score per residue for model 9

- Molecule 1: Gag protein



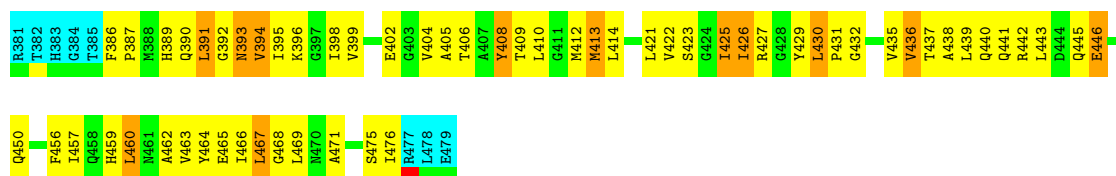
- Molecule 1: Gag protein



4.2.10 Score per residue for model 10

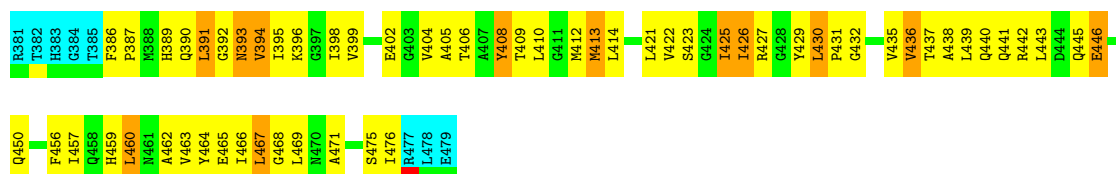
- Molecule 1: Gag protein

Chain A: 32% 47% 12% 8%



• Molecule 1: Gag protein

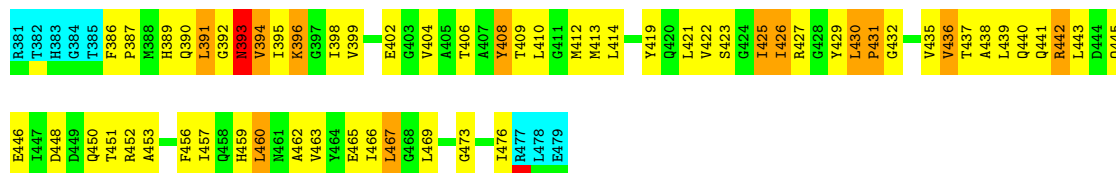
Chain B: 32% 47% 12% 8%



4.2.11 Score per residue for model 11

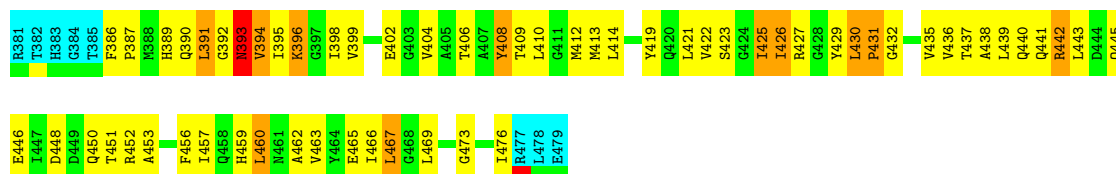
• Molecule 1: Gag protein

Chain A: 31% 47% 12% • 8%



• Molecule 1: Gag protein

Chain B: 31% 48% 11% • 8%



4.2.12 Score per residue for model 12

• Molecule 1: Gag protein

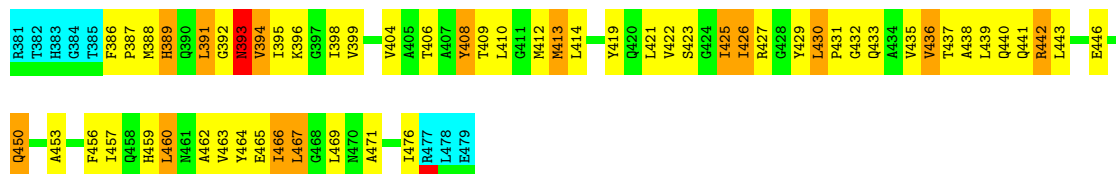
Chain A: 32% 44% 15% 8%





• Molecule 1: Gag protein

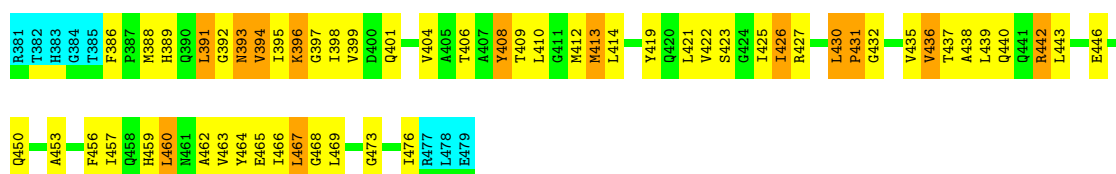
Chain B: 34% 42% 14% 8%



4.2.13 Score per residue for model 13

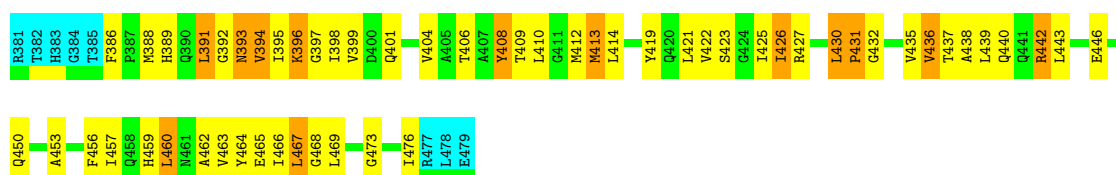
• Molecule 1: Gag protein

Chain A: 35% 43% 13% 8%



• Molecule 1: Gag protein

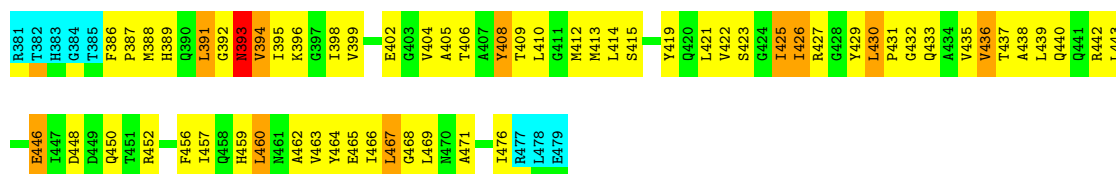
Chain B: 35% 43% 13% 8%



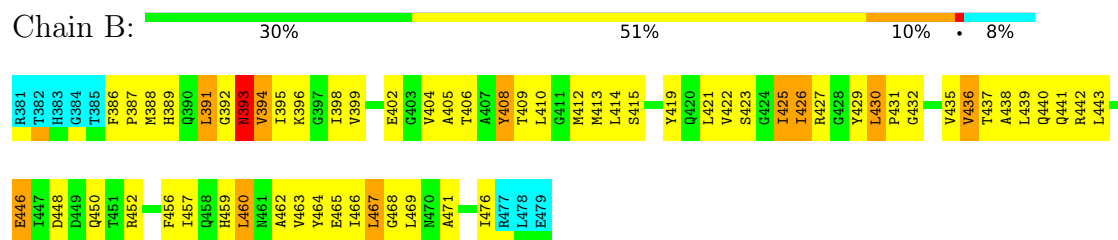
4.2.14 Score per residue for model 14

• Molecule 1: Gag protein

Chain A: 30% 51% 10% 8%

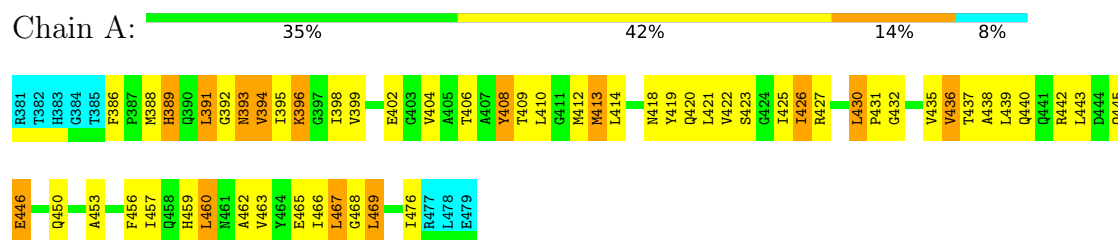


• Molecule 1: Gag protein

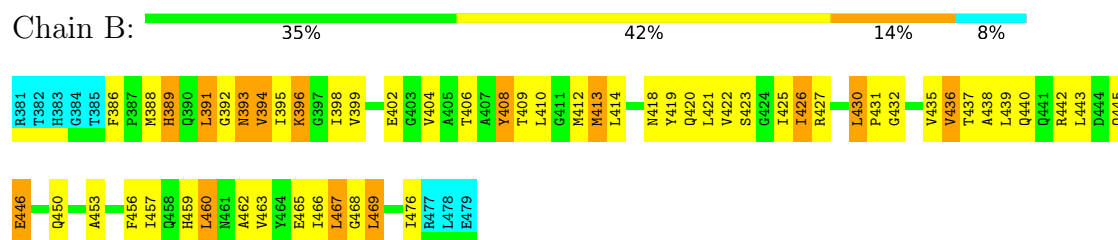


4.2.15 Score per residue for model 15

- Molecule 1: Gag protein

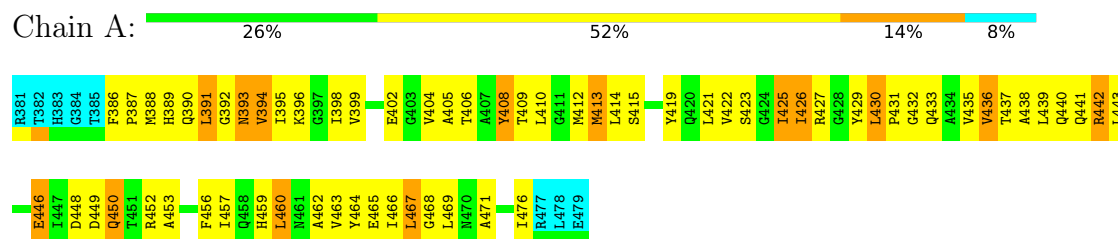


- Molecule 1: Gag protein

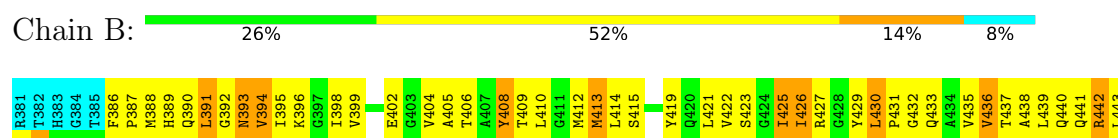


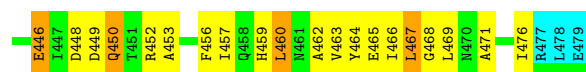
4.2.16 Score per residue for model 16

- Molecule 1: Gag protein



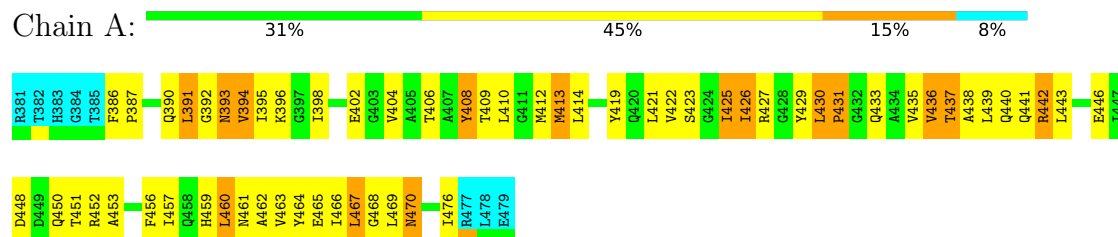
- Molecule 1: Gag protein



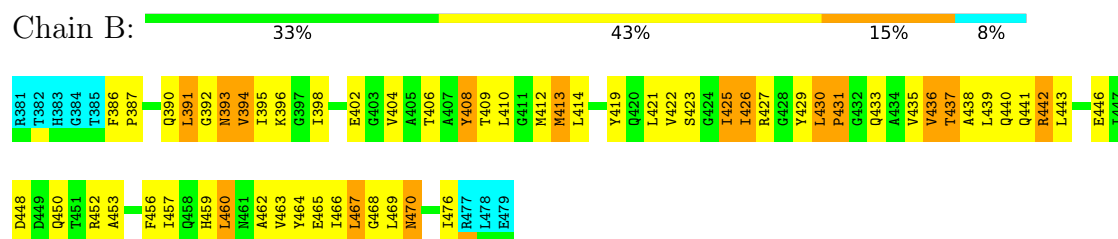


4.2.17 Score per residue for model 17

- Molecule 1: Gag protein

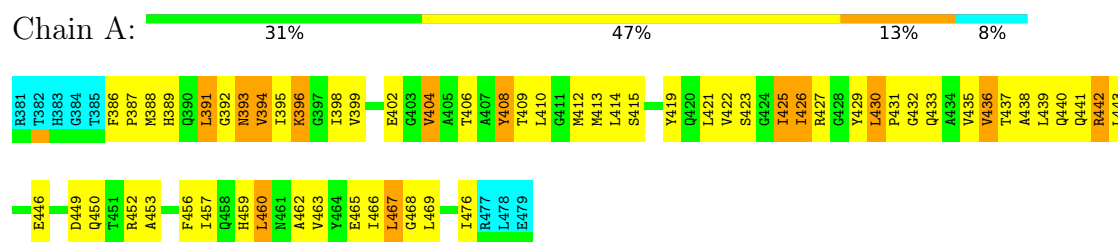


- Molecule 1: Gag protein

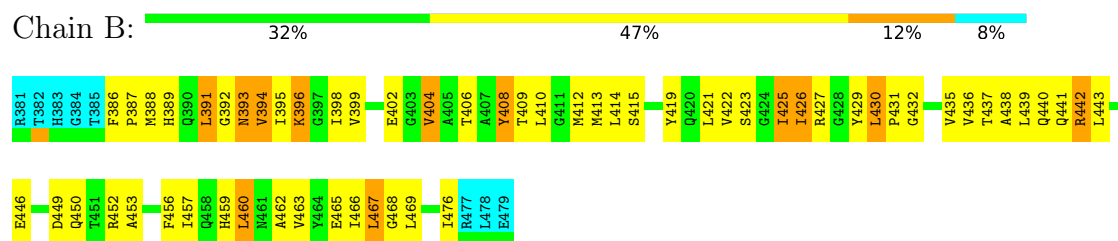


4.2.18 Score per residue for model 18

- Molecule 1: Gag protein

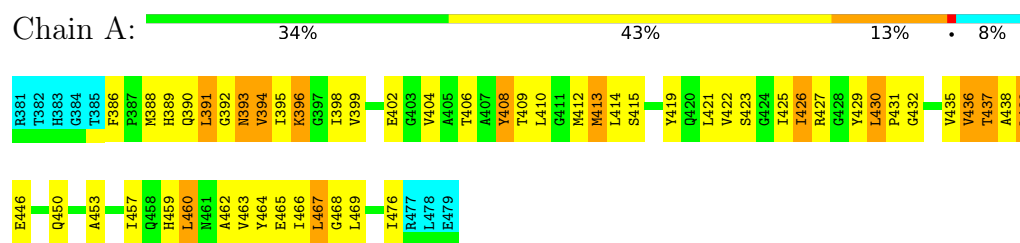


- Molecule 1: Gag protein

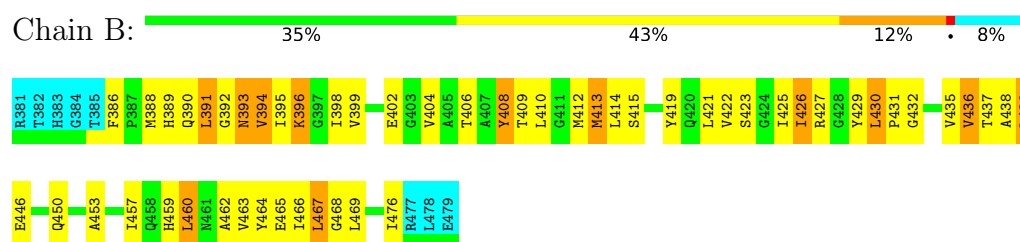


4.2.19 Score per residue for model 19

- Molecule 1: Gag protein

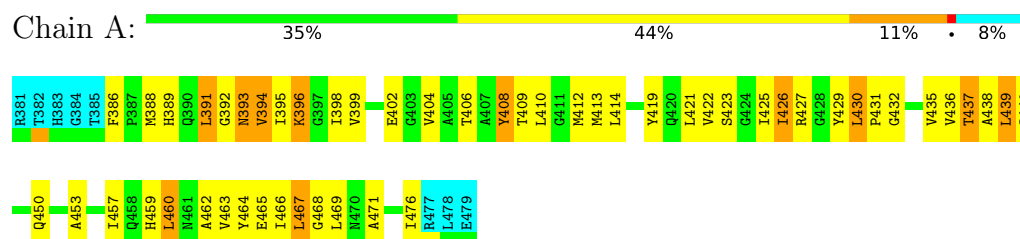


- Molecule 1: Gag protein

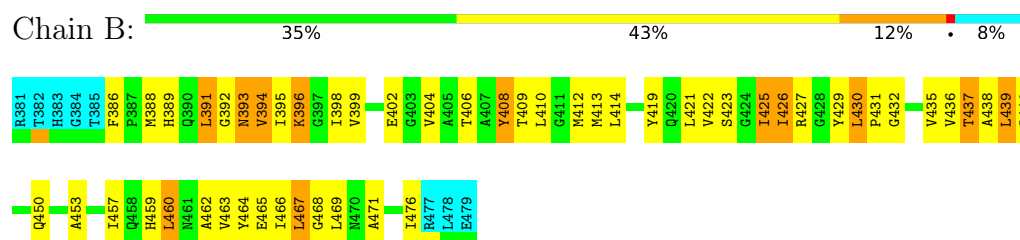


4.2.20 Score per residue for model 20

- Molecule 1: Gag protein



- Molecule 1: Gag protein



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 20 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	

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	4
Total number of shifts	2512
Number of shifts mapped to atoms	2512
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%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.64±0.02	0±0/711 (0.0± 0.0%)	1.00±0.02	0±1/964 (0.0± 0.1%)
1	B	0.64±0.02	0±0/711 (0.0± 0.0%)	1.00±0.02	0±1/964 (0.0± 0.1%)
All	All	0.64	0/28440 (0.0%)	1.00	11/38560 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
1	B	0.0±0.0	0.1±0.3
All	All	0	4

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	386	PHE	CA-C-N	6.00	125.48	119.24	7	1
1	B	386	PHE	C-N-CA	6.00	125.48	119.24	7	1
1	A	386	PHE	CA-C-N	5.93	125.40	119.24	7	1
1	A	386	PHE	C-N-CA	5.93	125.40	119.24	7	1
1	A	393	ASN	CA-CB-CG	5.32	117.92	112.60	5	3
1	B	393	ASN	CA-CB-CG	5.27	117.87	112.60	5	4

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	442	ARG	Sidechain	2
1	B	442	ARG	Sidechain	2

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	701	704	702	56±6
1	B	701	704	702	56±6
All	All	28040	28160	28080	2158

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 38.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:413:MET:SD	1:A:414:LEU:HG	0.85	2.11	4	20
1:B:413:MET:SD	1:B:414:LEU:HG	0.85	2.11	4	20
1:A:398:ILE:HD13	1:A:410:LEU:HD12	0.81	1.52	19	20
1:B:439:LEU:HD23	1:B:442:ARG:NH2	0.81	1.89	19	2
1:A:439:LEU:HD23	1:A:442:ARG:NH2	0.81	1.89	19	2
1:B:398:ILE:HD13	1:B:410:LEU:HD12	0.81	1.52	19	20
1:A:386:PHE:CD1	1:A:414:LEU:HD22	0.77	2.14	6	20
1:B:386:PHE:CD1	1:B:414:LEU:HD22	0.76	2.14	6	20
1:A:398:ILE:CD1	1:A:410:LEU:HD12	0.73	2.13	19	20
1:B:438:ALA:O	1:B:442:ARG:HG2	0.73	1.83	10	9
1:A:438:ALA:O	1:A:442:ARG:HG2	0.73	1.83	10	9
1:B:398:ILE:CD1	1:B:410:LEU:HD12	0.72	2.13	19	20
1:B:438:ALA:HB3	1:B:463:VAL:HG13	0.72	1.62	4	20
1:A:438:ALA:HB3	1:A:463:VAL:HG13	0.72	1.62	4	20
1:A:431:PRO:CD	1:A:435:VAL:HG11	0.72	2.15	17	6
1:B:431:PRO:CD	1:B:435:VAL:HG11	0.71	2.15	17	6
1:A:431:PRO:HD2	1:A:435:VAL:HG11	0.71	1.62	5	6
1:B:388:MET:SD	1:B:394:VAL:HG13	0.71	2.26	1	5
1:B:423:SER:O	1:B:427:ARG:HB2	0.71	1.86	13	20
1:B:431:PRO:HD2	1:B:435:VAL:HG11	0.70	1.62	14	6
1:B:467:LEU:CD1	1:B:469:LEU:HG	0.70	2.17	10	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:423:SER:O	1:A:427:ARG:HB2	0.70	1.86	8	20
1:B:386:PHE:CE2	1:B:394:VAL:HG12	0.70	2.22	19	19
1:A:389:HIS:CG	1:A:393:ASN:HB2	0.70	2.22	7	11
1:A:386:PHE:CE2	1:A:394:VAL:HG12	0.69	2.22	19	19
1:A:388:MET:SD	1:A:394:VAL:HG13	0.69	2.26	1	5
1:A:467:LEU:CD1	1:A:469:LEU:HG	0.69	2.16	10	20
1:B:389:HIS:CG	1:B:393:ASN:HB2	0.69	2.22	7	11
1:B:442:ARG:CZ	1:B:459:HIS:HB3	0.69	2.17	20	2
1:B:386:PHE:CZ	1:B:394:VAL:HG12	0.68	2.24	16	7
1:A:435:VAL:HG23	1:A:463:VAL:HG11	0.68	1.65	14	20
1:A:386:PHE:CZ	1:A:394:VAL:HG12	0.68	2.23	1	7
1:A:442:ARG:CZ	1:A:459:HIS:HB3	0.68	2.17	19	2
1:B:435:VAL:HG23	1:B:463:VAL:HG11	0.68	1.66	12	20
1:B:459:HIS:O	1:B:463:VAL:HG23	0.66	1.91	5	18
1:A:414:LEU:HD21	1:B:398:ILE:HG12	0.66	1.66	6	20
1:A:410:LEU:HD13	1:B:410:LEU:HD13	0.66	1.67	19	9
1:A:459:HIS:O	1:A:463:VAL:HG23	0.66	1.91	17	18
1:A:439:LEU:O	1:A:443:LEU:HG	0.66	1.90	19	20
1:A:396:LYS:HG3	1:A:429:TYR:CE1	0.66	2.25	4	4
1:B:439:LEU:O	1:B:443:LEU:HG	0.65	1.90	19	20
1:A:398:ILE:HG12	1:B:414:LEU:HD21	0.65	1.67	6	20
1:A:460:LEU:O	1:A:463:VAL:HB	0.64	1.92	19	20
1:B:396:LYS:HG3	1:B:429:TYR:CE1	0.64	2.26	4	6
1:B:460:LEU:O	1:B:463:VAL:HB	0.64	1.92	19	20
1:A:439:LEU:HA	1:A:442:ARG:CZ	0.64	2.23	20	2
1:B:464:TYR:CE2	1:B:471:ALA:HA	0.63	2.28	7	8
1:A:464:TYR:CE2	1:A:471:ALA:HA	0.63	2.28	7	8
1:A:406:THR:O	1:A:410:LEU:HG	0.63	1.94	6	20
1:B:406:THR:O	1:B:410:LEU:HG	0.63	1.94	6	20
1:B:439:LEU:HA	1:B:442:ARG:CZ	0.63	2.23	20	2
1:B:439:LEU:HD23	1:B:442:ARG:CZ	0.62	2.24	19	2
1:A:439:LEU:HD23	1:A:442:ARG:CZ	0.62	2.24	19	2
1:A:410:LEU:HA	1:A:413:MET:SD	0.61	2.35	17	19
1:B:410:LEU:HA	1:B:413:MET:SD	0.61	2.35	17	18
1:B:438:ALA:O	1:B:442:ARG:HD2	0.60	1.96	9	6
1:A:438:ALA:O	1:A:442:ARG:HD2	0.60	1.95	9	6
1:B:388:MET:HE1	1:B:415:SER:HB2	0.60	1.73	16	2
1:A:391:LEU:HG	1:A:392:GLY:N	0.60	2.12	16	18
1:A:467:LEU:HD13	1:A:469:LEU:HG	0.60	1.73	10	20
1:B:396:LYS:HG3	1:B:429:TYR:CZ	0.59	2.32	10	10
1:B:392:GLY:HA3	1:B:395:ILE:HD13	0.59	1.74	19	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:468:GLY:O	1:B:476:ILE:HG13	0.59	1.98	14	18
1:A:396:LYS:HG3	1:A:429:TYR:CZ	0.59	2.33	2	10
1:A:388:MET:HE1	1:A:415:SER:HB2	0.59	1.73	16	2
1:B:391:LEU:HG	1:B:392:GLY:N	0.59	2.12	16	18
1:B:442:ARG:HG3	1:B:459:HIS:CG	0.59	2.32	11	6
1:B:431:PRO:HG2	1:B:469:LEU:CD1	0.59	2.27	14	6
1:A:468:GLY:O	1:A:476:ILE:HG13	0.59	1.98	14	18
1:A:431:PRO:HG2	1:A:469:LEU:CD1	0.59	2.27	14	6
1:B:467:LEU:HD13	1:B:469:LEU:HG	0.59	1.72	10	20
1:A:392:GLY:HA3	1:A:395:ILE:HD13	0.59	1.74	19	17
1:A:442:ARG:HG3	1:A:459:HIS:CG	0.58	2.33	11	6
1:B:439:LEU:HD23	1:B:442:ARG:HH22	0.58	1.59	20	2
1:B:394:VAL:HG23	1:B:398:ILE:HD12	0.58	1.75	3	13
1:A:394:VAL:HG23	1:A:398:ILE:HD12	0.57	1.75	3	13
1:B:404:VAL:O	1:B:408:TYR:HB2	0.57	1.99	11	20
1:A:404:VAL:O	1:A:408:TYR:HB2	0.57	1.99	10	20
1:A:439:LEU:HD23	1:A:442:ARG:HH22	0.57	1.59	20	2
1:A:442:ARG:HG3	1:A:442:ARG:HH11	0.57	1.60	19	2
1:B:388:MET:O	1:B:388:MET:HG3	0.56	2.01	7	1
1:A:388:MET:O	1:A:388:MET:HG3	0.56	2.00	7	1
1:B:449:ASP:O	1:B:452:ARG:HG2	0.56	2.01	18	1
1:B:442:ARG:HG3	1:B:442:ARG:HH11	0.56	1.59	20	2
1:B:427:ARG:HA	1:B:430:LEU:HD23	0.55	1.77	1	14
1:B:409:THR:HG22	1:B:410:LEU:HD23	0.55	1.79	15	20
1:A:449:ASP:O	1:A:452:ARG:HG2	0.55	2.01	18	1
1:A:427:ARG:HA	1:A:430:LEU:HD23	0.55	1.77	1	14
1:A:395:ILE:HG23	1:A:426:ILE:HD13	0.55	1.79	4	20
1:A:426:ILE:HG22	1:A:430:LEU:HD22	0.55	1.77	18	14
1:A:409:THR:HG22	1:A:410:LEU:HD23	0.54	1.79	15	20
1:B:448:ASP:O	1:B:452:ARG:HG3	0.54	2.02	1	5
1:A:470:ASN:C	1:A:470:ASN:HD22	0.54	2.11	17	1
1:A:448:ASP:O	1:A:452:ARG:HG3	0.54	2.02	1	5
1:B:442:ARG:HH11	1:B:442:ARG:CG	0.54	2.15	19	2
1:B:426:ILE:HG22	1:B:430:LEU:HD22	0.54	1.77	18	14
1:B:462:ALA:O	1:B:466:ILE:HD12	0.54	2.03	3	20
1:A:442:ARG:HH11	1:A:442:ARG:CG	0.54	2.15	19	2
1:B:470:ASN:HD22	1:B:470:ASN:C	0.53	2.11	17	1
1:B:395:ILE:HG23	1:B:426:ILE:HD13	0.53	1.79	4	20
1:A:442:ARG:NH1	1:A:459:HIS:HB3	0.53	2.18	19	2
1:A:462:ALA:O	1:A:466:ILE:HD12	0.53	2.03	3	20
1:A:389:HIS:CE1	1:A:393:ASN:HA	0.53	2.39	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:396:LYS:O	1:B:399:VAL:HG22	0.52	2.04	18	16
1:B:389:HIS:O	1:B:390:GLN:HG2	0.52	2.04	11	1
1:A:442:ARG:HH21	1:A:463:VAL:CG2	0.52	2.18	20	2
1:A:396:LYS:O	1:A:399:VAL:HG22	0.52	2.04	18	16
1:B:442:ARG:NH1	1:B:459:HIS:HB3	0.52	2.18	19	2
1:A:389:HIS:O	1:A:390:GLN:HG2	0.52	2.05	11	1
1:B:442:ARG:HH21	1:B:463:VAL:CG2	0.52	2.18	20	2
1:A:395:ILE:HG21	1:A:425:ILE:HG22	0.52	1.81	7	13
1:B:389:HIS:CE1	1:B:393:ASN:HA	0.51	2.40	5	9
1:B:419:TYR:HB2	1:B:456:PHE:CE2	0.51	2.40	7	5
1:A:387:PRO:HG2	1:B:393:ASN:OD1	0.51	2.05	3	4
1:A:388:MET:SD	1:A:392:GLY:HA2	0.51	2.46	1	2
1:B:419:TYR:CD1	1:B:453:ALA:HB2	0.51	2.40	20	16
1:B:389:HIS:CD2	1:B:393:ASN:HB2	0.51	2.41	15	7
1:B:388:MET:SD	1:B:392:GLY:HA2	0.51	2.46	1	2
1:B:395:ILE:HG21	1:B:425:ILE:HG22	0.51	1.81	7	15
1:B:438:ALA:O	1:B:441:GLN:HB2	0.51	2.06	12	12
1:A:419:TYR:HB2	1:A:456:PHE:CE2	0.51	2.40	7	5
1:A:389:HIS:CD2	1:A:393:ASN:HB2	0.51	2.40	20	7
1:A:419:TYR:CD1	1:A:453:ALA:HB2	0.51	2.40	20	16
1:A:438:ALA:O	1:A:441:GLN:HB2	0.51	2.06	12	11
1:A:393:ASN:OD1	1:B:387:PRO:HG2	0.50	2.05	3	4
1:B:435:VAL:CG2	1:B:463:VAL:HG11	0.50	2.35	12	16
1:A:435:VAL:CG2	1:A:463:VAL:HG11	0.50	2.35	12	14
1:B:423:SER:HB3	1:B:456:PHE:CZ	0.50	2.42	8	15
1:B:394:VAL:HG23	1:B:398:ILE:CD1	0.50	2.37	4	7
1:A:394:VAL:HG23	1:A:398:ILE:CD1	0.50	2.37	4	8
1:A:389:HIS:N	1:A:393:ASN:HB3	0.50	2.22	9	3
1:B:389:HIS:N	1:B:393:ASN:HB3	0.50	2.21	9	3
1:A:423:SER:HB3	1:A:456:PHE:CZ	0.50	2.42	8	16
1:A:433:GLN:O	1:A:436:VAL:HG13	0.50	2.07	7	10
1:B:389:HIS:ND1	1:B:393:ASN:HA	0.50	2.22	18	5
1:B:433:GLN:O	1:B:436:VAL:HG13	0.49	2.07	7	8
1:A:394:VAL:HG11	1:A:414:LEU:CD1	0.49	2.38	6	4
1:A:405:ALA:HB1	1:A:457:ILE:HG23	0.49	1.84	7	4
1:B:394:VAL:HG11	1:B:414:LEU:CD1	0.48	2.38	6	4
1:B:439:LEU:C	1:B:439:LEU:HD22	0.48	2.33	19	2
1:A:388:MET:HA	1:A:393:ASN:HB3	0.48	1.84	20	6
1:B:388:MET:HA	1:B:393:ASN:HB3	0.48	1.85	20	6
1:A:439:LEU:C	1:A:439:LEU:HD22	0.48	2.33	20	2
1:A:389:HIS:ND1	1:A:393:ASN:HA	0.48	2.23	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:414:LEU:HA	1:B:401:GLN:NE2	0.48	2.23	5	1
1:B:405:ALA:HB1	1:B:457:ILE:HG23	0.48	1.84	7	4
1:B:437:THR:O	1:B:441:GLN:HG3	0.48	2.08	17	1
1:A:442:ARG:NH1	1:A:459:HIS:CB	0.48	2.77	19	2
1:A:401:GLN:NE2	1:B:414:LEU:HA	0.48	2.24	5	1
1:B:442:ARG:NH1	1:B:459:HIS:CB	0.48	2.77	20	2
1:A:437:THR:O	1:A:441:GLN:HG3	0.48	2.09	17	1
1:A:391:LEU:CG	1:A:392:GLY:N	0.48	2.75	16	8
1:B:442:ARG:HG3	1:B:459:HIS:HB3	0.48	1.86	18	10
1:A:392:GLY:CA	1:A:395:ILE:HD13	0.48	2.39	15	6
1:B:394:VAL:HG22	1:B:395:ILE:HD12	0.48	1.86	1	4
1:B:391:LEU:CG	1:B:392:GLY:N	0.48	2.76	16	8
1:A:431:PRO:N	1:A:435:VAL:HG11	0.48	2.24	17	5
1:B:443:LEU:O	1:B:446:GLU:HB2	0.47	2.09	14	3
1:B:397:GLY:O	1:B:401:GLN:HG3	0.47	2.09	7	3
1:B:432:GLY:O	1:B:435:VAL:HG12	0.47	2.09	1	15
1:B:467:LEU:HD11	1:B:469:LEU:HG	0.47	1.86	9	9
1:A:390:GLN:HG2	1:A:390:GLN:O	0.47	2.10	19	1
1:A:386:PHE:CD2	1:A:386:PHE:C	0.47	2.93	19	10
1:A:443:LEU:O	1:A:446:GLU:HB2	0.47	2.09	14	3
1:A:442:ARG:HG3	1:A:459:HIS:HB3	0.47	1.85	18	8
1:B:392:GLY:CA	1:B:395:ILE:HD13	0.47	2.39	15	6
1:B:423:SER:HB2	1:B:456:PHE:CZ	0.47	2.45	18	2
1:A:442:ARG:HH21	1:A:463:VAL:HG23	0.47	1.70	20	2
1:A:394:VAL:HG22	1:A:395:ILE:HD12	0.47	1.86	1	3
1:B:442:ARG:CZ	1:B:459:HIS:CB	0.47	2.92	20	2
1:B:408:TYR:OH	1:B:423:SER:HA	0.47	2.09	7	14
1:B:431:PRO:N	1:B:435:VAL:HG11	0.47	2.24	17	4
1:A:395:ILE:H	1:A:395:ILE:HD12	0.47	1.69	3	14
1:B:431:PRO:HG3	1:B:473:GLY:O	0.47	2.10	11	2
1:A:432:GLY:O	1:A:435:VAL:HG12	0.46	2.11	15	14
1:A:397:GLY:O	1:A:401:GLN:HG3	0.46	2.09	7	3
1:A:423:SER:HB2	1:A:456:PHE:CZ	0.46	2.45	18	2
1:B:386:PHE:HD1	1:B:414:LEU:HD22	0.46	1.66	6	1
1:B:450:GLN:O	1:B:453:ALA:HB3	0.46	2.10	6	2
1:B:386:PHE:CD2	1:B:386:PHE:C	0.46	2.93	19	11
1:B:408:TYR:HB3	1:B:457:ILE:CG1	0.46	2.40	6	20
1:B:430:LEU:HD12	1:B:431:PRO:HD2	0.46	1.87	10	6
1:A:450:GLN:O	1:A:453:ALA:HB3	0.46	2.10	6	2
1:A:408:TYR:OH	1:A:423:SER:HA	0.46	2.09	7	14
1:A:430:LEU:HD12	1:A:431:PRO:HD2	0.46	1.87	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:439:LEU:HD23	1:A:442:ARG:NH1	0.46	2.26	19	2
1:A:398:ILE:HG12	1:B:413:MET:HE1	0.46	1.87	12	9
1:A:414:LEU:HD21	1:B:398:ILE:CG1	0.46	2.40	6	2
1:A:435:VAL:HG23	1:A:463:VAL:CG1	0.46	2.40	12	10
1:A:389:HIS:H	1:A:393:ASN:HB3	0.46	1.71	12	1
1:A:404:VAL:HG11	1:A:430:LEU:HA	0.46	1.87	1	11
1:A:413:MET:HE1	1:B:398:ILE:HG12	0.46	1.87	12	8
1:A:467:LEU:HD11	1:A:469:LEU:HG	0.46	1.86	9	8
1:A:408:TYR:HB3	1:A:457:ILE:CG1	0.45	2.40	6	20
1:B:389:HIS:H	1:B:393:ASN:HB3	0.45	1.72	12	1
1:B:390:GLN:O	1:B:390:GLN:HG2	0.45	2.10	19	1
1:B:395:ILE:HD12	1:B:395:ILE:H	0.45	1.70	3	15
1:A:431:PRO:HG3	1:A:473:GLY:O	0.45	2.11	11	2
1:A:442:ARG:CZ	1:A:459:HIS:CB	0.45	2.92	20	2
1:B:439:LEU:CD2	1:B:442:ARG:NH1	0.45	2.79	20	2
1:B:442:ARG:HH21	1:B:463:VAL:HG23	0.45	1.70	20	2
1:A:439:LEU:CD2	1:A:442:ARG:NH1	0.45	2.79	20	2
1:A:431:PRO:HG2	1:A:469:LEU:HD11	0.45	1.89	9	2
1:A:441:GLN:O	1:A:445:GLN:HG2	0.45	2.12	7	1
1:A:386:PHE:CZ	1:B:386:PHE:CZ	0.45	3.04	19	2
1:A:438:ALA:CB	1:A:463:VAL:HG13	0.45	2.40	4	13
1:B:404:VAL:HG11	1:B:430:LEU:HA	0.45	1.88	1	10
1:B:441:GLN:O	1:B:445:GLN:HG2	0.45	2.12	7	1
1:A:388:MET:SD	1:A:415:SER:HB2	0.45	2.52	14	1
1:A:435:VAL:HA	1:A:463:VAL:CG1	0.45	2.41	9	5
1:B:435:VAL:HA	1:B:463:VAL:CG1	0.45	2.41	9	6
1:A:464:TYR:CD1	1:A:469:LEU:HB2	0.45	2.46	9	5
1:B:431:PRO:HG2	1:B:469:LEU:HD11	0.45	1.89	9	2
1:B:464:TYR:CD1	1:B:469:LEU:HB2	0.45	2.47	9	8
1:A:386:PHE:HD1	1:A:414:LEU:HD22	0.45	1.65	6	1
1:B:388:MET:SD	1:B:415:SER:HB2	0.45	2.52	14	1
1:B:439:LEU:HD23	1:B:442:ARG:NH1	0.45	2.26	19	2
1:B:429:TYR:N	1:B:429:TYR:CD2	0.45	2.84	19	3
1:B:395:ILE:HG22	1:B:429:TYR:HD1	0.44	1.72	1	6
1:B:435:VAL:HG23	1:B:463:VAL:CG1	0.44	2.40	12	6
1:A:396:LYS:HD2	1:A:429:TYR:CE1	0.44	2.47	19	1
1:A:393:ASN:OD1	1:A:393:ASN:C	0.44	2.61	12	6
1:A:437:THR:O	1:A:441:GLN:HG2	0.44	2.12	20	2
1:A:395:ILE:HG22	1:A:429:TYR:HD1	0.44	1.72	1	5
1:A:408:TYR:HB3	1:A:457:ILE:HG13	0.44	1.90	6	13
1:B:396:LYS:HD2	1:B:429:TYR:CE1	0.44	2.47	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:442:ARG:NH2	1:A:460:LEU:HA	0.44	2.27	19	2
1:B:442:ARG:NH2	1:B:460:LEU:HA	0.44	2.27	19	2
1:B:438:ALA:O	1:B:442:ARG:HG3	0.44	2.13	5	3
1:B:442:ARG:NH1	1:B:462:ALA:HB1	0.44	2.27	5	1
1:A:404:VAL:HG11	1:A:430:LEU:HD13	0.44	1.90	1	4
1:A:464:TYR:HA	1:A:469:LEU:HB2	0.44	1.90	5	9
1:B:437:THR:O	1:B:441:GLN:HG2	0.44	2.12	20	1
1:B:438:ALA:CB	1:B:463:VAL:HG13	0.44	2.40	4	13
1:A:438:ALA:O	1:A:442:ARG:HG3	0.44	2.13	5	3
1:B:476:ILE:HD12	1:B:476:ILE:C	0.44	2.38	11	1
1:B:408:TYR:HB3	1:B:457:ILE:HG13	0.44	1.90	6	11
1:A:429:TYR:CD2	1:A:429:TYR:N	0.44	2.84	19	3
1:B:393:ASN:OD1	1:B:393:ASN:C	0.43	2.61	14	6
1:B:442:ARG:HB3	1:B:459:HIS:CG	0.43	2.49	10	1
1:A:442:ARG:NH1	1:A:462:ALA:HB1	0.43	2.27	5	1
1:A:476:ILE:HD12	1:A:476:ILE:C	0.43	2.38	11	1
1:A:459:HIS:O	1:A:462:ALA:HB3	0.43	2.13	19	2
1:B:443:LEU:O	1:B:446:GLU:HB3	0.43	2.13	15	1
1:B:404:VAL:HG11	1:B:430:LEU:HD13	0.43	1.90	1	3
1:B:461:ASN:HA	1:B:464:TYR:CD2	0.43	2.48	7	1
1:A:398:ILE:CG1	1:B:414:LEU:HD21	0.43	2.42	6	2
1:B:448:ASP:HB2	1:B:451:THR:OG1	0.43	2.13	11	3
1:A:461:ASN:HA	1:A:464:TYR:CD2	0.43	2.48	7	1
1:B:396:LYS:H	1:B:396:LYS:CD	0.43	2.26	10	8
1:A:396:LYS:H	1:A:396:LYS:CD	0.43	2.26	10	6
1:B:464:TYR:HA	1:B:469:LEU:HB2	0.43	1.91	17	7
1:B:431:PRO:HD2	1:B:435:VAL:HG21	0.43	1.90	17	1
1:A:432:GLY:O	1:A:436:VAL:HG12	0.43	2.14	1	10
1:A:394:VAL:HG11	1:A:414:LEU:HD13	0.43	1.91	18	3
1:A:442:ARG:HG3	1:A:459:HIS:ND1	0.42	2.29	9	3
1:A:388:MET:C	1:A:393:ASN:HB3	0.42	2.39	14	2
1:A:448:ASP:HB2	1:A:451:THR:OG1	0.42	2.13	11	5
1:B:442:ARG:HG3	1:B:459:HIS:ND1	0.42	2.29	9	2
1:A:442:ARG:HB3	1:A:459:HIS:CG	0.42	2.49	10	1
1:B:432:GLY:O	1:B:436:VAL:HG12	0.42	2.15	5	9
1:A:386:PHE:HZ	1:B:386:PHE:CZ	0.42	2.33	19	2
1:A:435:VAL:HG13	1:A:436:VAL:N	0.42	2.30	17	1
1:B:394:VAL:HG11	1:B:414:LEU:HD13	0.42	1.91	18	2
1:A:442:ARG:HG3	1:A:459:HIS:CB	0.42	2.44	18	2
1:B:445:GLN:O	1:B:446:GLU:C	0.42	2.63	10	1
1:B:388:MET:C	1:B:393:ASN:HB3	0.42	2.40	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:445:GLN:O	1:A:446:GLU:C	0.42	2.63	10	1
1:A:442:ARG:CD	1:A:459:HIS:HB3	0.42	2.45	20	2
1:B:439:LEU:CD1	1:B:443:LEU:HD11	0.42	2.44	8	1
1:B:442:ARG:HG3	1:B:459:HIS:CB	0.42	2.44	18	2
1:B:394:VAL:CG2	1:B:395:ILE:N	0.42	2.83	16	1
1:A:446:GLU:O	1:A:446:GLU:HG3	0.41	2.15	10	1
1:A:386:PHE:CZ	1:B:386:PHE:HZ	0.41	2.33	19	2
1:A:443:LEU:O	1:A:446:GLU:HB3	0.41	2.14	15	1
1:B:459:HIS:O	1:B:462:ALA:HB3	0.41	2.14	19	2
1:B:476:ILE:C	1:B:476:ILE:HD12	0.41	2.40	8	2
1:A:438:ALA:HB1	1:A:466:ILE:HD13	0.41	1.92	11	1
1:B:435:VAL:HG13	1:B:436:VAL:N	0.41	2.30	17	1
1:A:439:LEU:O	1:A:439:LEU:HD22	0.41	2.15	19	2
1:A:449:ASP:CG	1:A:450:GLN:N	0.41	2.79	16	1
1:A:388:MET:HE1	1:A:415:SER:HB3	0.41	1.90	18	1
1:B:388:MET:HE1	1:B:415:SER:HB3	0.41	1.90	18	1
1:B:446:GLU:O	1:B:446:GLU:HG3	0.41	2.15	10	1
1:A:431:PRO:HD2	1:A:435:VAL:HG21	0.41	1.90	17	1
1:A:449:ASP:HA	1:A:452:ARG:CZ	0.41	2.46	5	1
1:A:439:LEU:CD1	1:A:443:LEU:HD11	0.41	2.44	8	1
1:A:394:VAL:CG2	1:A:395:ILE:N	0.41	2.83	16	1
1:B:439:LEU:O	1:B:439:LEU:HD22	0.41	2.15	19	2
1:A:419:TYR:HA	1:A:422:VAL:CG2	0.41	2.46	5	1
1:B:426:ILE:O	1:B:430:LEU:N	0.41	2.54	18	5
1:B:439:LEU:HA	1:B:442:ARG:NE	0.41	2.30	20	1
1:A:396:LYS:CD	1:A:396:LYS:H	0.41	2.28	2	2
1:A:450:GLN:C	1:A:450:GLN:HE21	0.41	2.23	7	1
1:A:476:ILE:C	1:A:476:ILE:HD12	0.41	2.40	8	2
1:B:427:ARG:NE	1:B:436:VAL:HG21	0.41	2.31	10	2
1:A:452:ARG:HG3	1:A:453:ALA:N	0.41	2.31	18	1
1:B:442:ARG:CD	1:B:459:HIS:HB3	0.41	2.45	20	2
1:B:449:ASP:CG	1:B:450:GLN:N	0.40	2.79	16	1
1:B:452:ARG:HG3	1:B:453:ALA:N	0.40	2.31	18	1
1:B:442:ARG:CG	1:B:442:ARG:NH1	0.40	2.81	19	2
1:B:389:HIS:CE1	1:B:393:ASN:HB2	0.40	2.51	4	1
1:B:388:MET:O	1:B:389:HIS:HB2	0.40	2.16	7	1
1:B:439:LEU:HD11	1:B:456:PHE:CE1	0.40	2.52	18	1
1:A:439:LEU:HA	1:A:442:ARG:NE	0.40	2.30	20	1
1:B:419:TYR:HA	1:B:422:VAL:CG2	0.40	2.46	5	1
1:B:395:ILE:HD12	1:B:395:ILE:N	0.40	2.32	15	1
1:A:461:ASN:O	1:A:464:TYR:HB2	0.40	2.17	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:426:ILE:O	1:A:430:LEU:N	0.40	2.54	9	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	91/99 (92%)	80±1 (88±2%)	7±1 (7±1%)	4±1 (4±1%)	3	27
1	B	91/99 (92%)	80±1 (88±2%)	7±1 (7±1%)	4±1 (4±1%)	3	27
All	All	3640/3960 (92%)	3214 (88%)	265 (7%)	161 (4%)	3	27

All 18 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	446	GLU	20
1	B	446	GLU	20
1	A	391	LEU	17
1	B	391	LEU	17
1	A	431	PRO	16
1	B	431	PRO	16
1	A	389	HIS	9
1	A	387	PRO	9
1	B	387	PRO	9
1	B	389	HIS	8
1	A	390	GLN	6
1	B	390	GLN	6
1	A	386	PHE	2
1	B	386	PHE	2
1	A	392	GLY	1
1	B	392	GLY	1
1	A	388	MET	1
1	B	388	MET	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	74/81 (91%)	54±1 (74±2%)	20±1 (26±2%)	2	22
1	B	74/81 (91%)	54±1 (74±2%)	20±1 (26±2%)	2	22
All	All	2960/3240 (91%)	2177 (74%)	783 (26%)	2	22

All 60 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	393	ASN	20
1	A	394	VAL	20
1	A	408	TYR	20
1	A	412	MET	20
1	A	421	LEU	20
1	A	422	VAL	20
1	A	426	ILE	20
1	A	430	LEU	20
1	A	436	VAL	20
1	A	437	THR	20
1	A	440	GLN	20
1	A	450	GLN	20
1	A	460	LEU	20
1	A	465	GLU	20
1	A	467	LEU	20
1	B	393	ASN	20
1	B	394	VAL	20
1	B	408	TYR	20
1	B	412	MET	20
1	B	421	LEU	20
1	B	422	VAL	20
1	B	426	ILE	20
1	B	430	LEU	20
1	B	436	VAL	20
1	B	437	THR	20
1	B	440	GLN	20
1	B	450	GLN	20
1	B	460	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	B	465	GLU	20
1	B	467	LEU	20
1	A	425	ILE	19
1	B	425	ILE	19
1	A	402	GLU	15
1	B	402	GLU	15
1	A	413	MET	14
1	A	442	ARG	14
1	B	442	ARG	14
1	B	413	MET	13
1	A	396	LYS	11
1	B	396	LYS	11
1	A	466	ILE	3
1	B	466	ILE	3
1	A	420	GLN	3
1	B	420	GLN	3
1	A	445	GLN	3
1	B	445	GLN	3
1	A	415	SER	2
1	B	415	SER	2
1	A	404	VAL	2
1	B	404	VAL	2
1	A	439	LEU	2
1	B	439	LEU	2
1	A	433	GLN	1
1	A	475	SER	1
1	B	433	GLN	1
1	B	475	SER	1
1	A	469	LEU	1
1	B	469	LEU	1
1	A	470	ASN	1
1	B	470	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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

The completeness of assignment taking into account all chemical shift lists is 41% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *13C-HPFV-381-477-27012015-chemical-shifts*

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	911
Number of shifts mapped to atoms	911
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	89	-0.57 ± 0.08	Should be checked
$^{13}\text{C}_\beta$	82	0.15 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

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 35%, i.e. 864 atoms were assigned a chemical shift out of a possible 2486. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	254/922 (28%)	171/380 (45%)	83/364 (23%)	0/178 (0%)
Sidechain	586/1420 (41%)	407/930 (44%)	179/434 (41%)	0/56 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	24/144 (17%)	24/68 (35%)	0/68 (0%)	0/8 (0%)
Overall	864/2486 (35%)	602/1378 (44%)	262/866 (30%)	0/242 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 33%, i.e. 911 atoms were assigned a chemical shift out of a possible 2726. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	268/1004 (27%)	179/414 (43%)	89/396 (22%)	0/194 (0%)
Sidechain	618/1562 (40%)	429/1020 (42%)	189/474 (40%)	0/68 (0%)
Aromatic	25/160 (16%)	25/76 (33%)	0/72 (0%)	0/12 (0%)
Overall	911/2726 (33%)	633/1510 (42%)	278/942 (30%)	0/274 (0%)

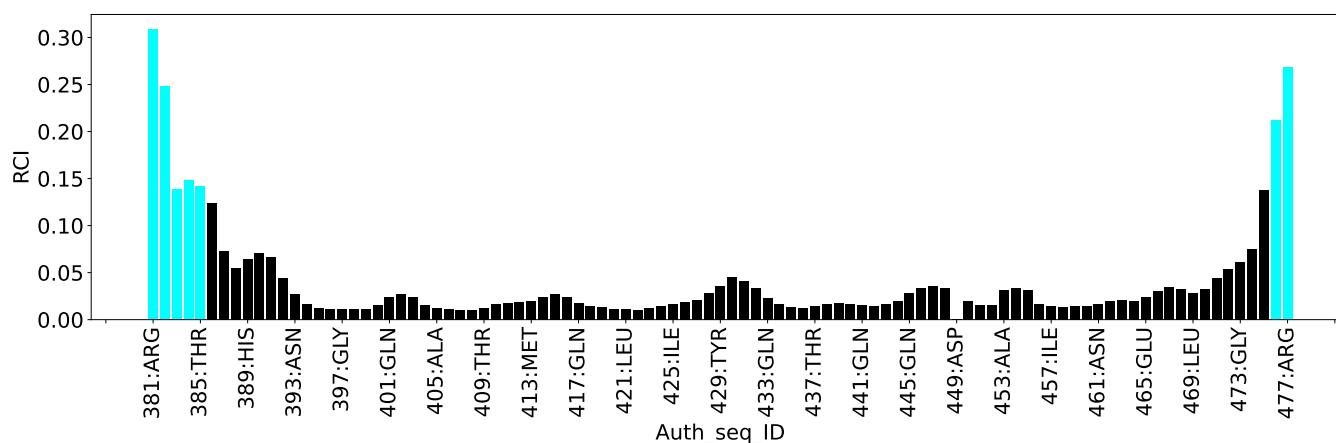
7.1.4 Statistically unusual chemical shifts [i](#)

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *15N-HPFV-381-477-chemical-shifts*

7.2.1 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	632
Number of shifts mapped to atoms	632
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

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	79	0.74 ± 0.31	Should be applied

7.2.3 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 25%, i.e. 623 atoms were assigned a chemical shift out of a possible 2486. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	244/922 (26%)	167/380 (44%)	0/364 (0%)	77/178 (43%)
Sidechain	370/1420 (26%)	356/930 (38%)	0/434 (0%)	14/56 (25%)
Aromatic	9/144 (6%)	9/68 (13%)	0/68 (0%)	0/8 (0%)
Overall	623/2486 (25%)	532/1378 (39%)	0/866 (0%)	91/242 (38%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 23%, i.e. 632 atoms were assigned a chemical shift out of a possible 2726. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	249/1004 (25%)	170/414 (41%)	0/396 (0%)	79/194 (41%)
Sidechain	374/1562 (24%)	360/1020 (35%)	0/474 (0%)	14/68 (21%)
Aromatic	9/160 (6%)	9/76 (12%)	0/72 (0%)	0/12 (0%)
Overall	632/2726 (23%)	539/1510 (36%)	0/942 (0%)	93/274 (34%)

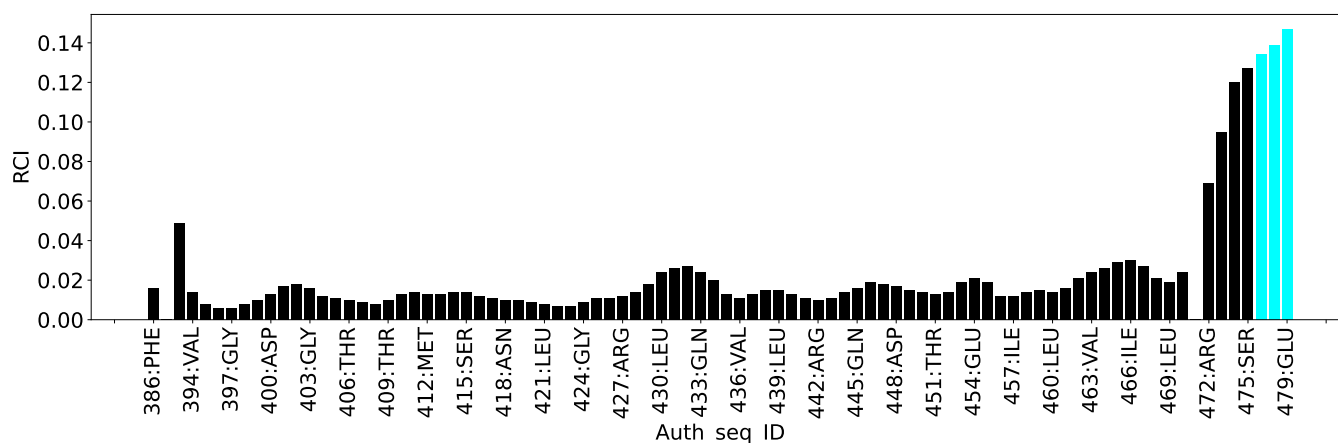
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *13C-ARO-HPFV-381-477-chemical-shifts*

7.3.1 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	151
Number of shifts mapped to atoms	151
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

7.3.2 Chemical shift referencing [i](#)

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

7.3.3 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 6%, i.e. 147 atoms were assigned a chemical shift out of a possible 2486. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	15/922 (2%)	15/380 (4%)	0/364 (0%)	0/178 (0%)
Sidechain	93/1420 (7%)	93/930 (10%)	0/434 (0%)	0/56 (0%)
Aromatic	39/144 (27%)	25/68 (37%)	14/68 (21%)	0/8 (0%)
Overall	147/2486 (6%)	133/1378 (10%)	14/866 (2%)	0/242 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 151 atoms were assigned a chemical shift out of a possible 2726. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	15/1004 (1%)	15/414 (4%)	0/396 (0%)	0/194 (0%)
Sidechain	95/1562 (6%)	95/1020 (9%)	0/474 (0%)	0/68 (0%)
Aromatic	41/160 (26%)	26/76 (34%)	15/72 (21%)	0/12 (0%)
Overall	151/2726 (6%)	136/1510 (9%)	15/942 (2%)	0/274 (0%)

7.3.4 Statistically unusual chemical shifts [i](#)

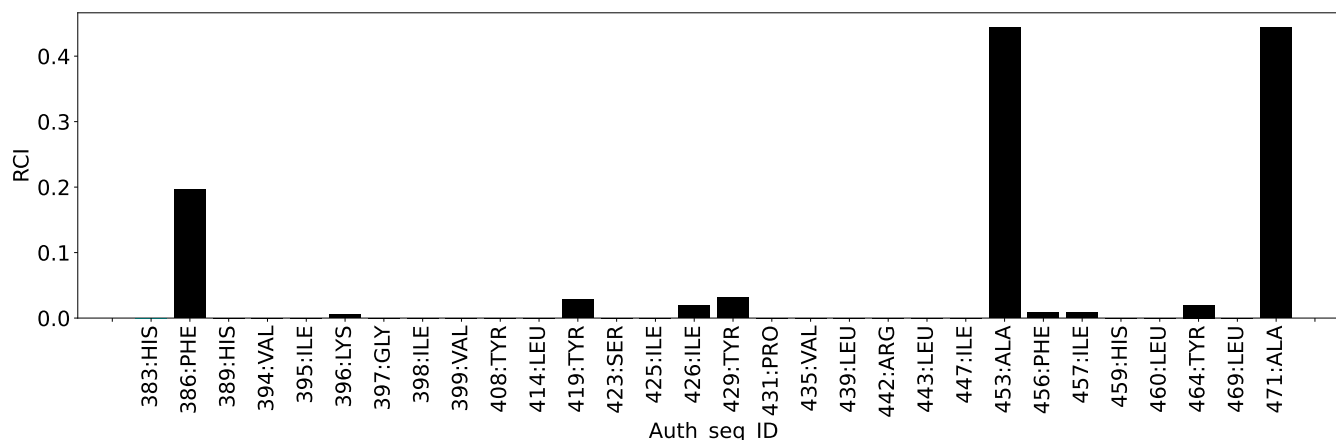
There are no statistically unusual chemical shifts.

7.3.5 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:



7.4 Chemical shift list 4

File name: working_cs.cif

Chemical shift list name: *13C-HPFV-381-477-D2O-chemical-shifts*

7.4.1 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	818
Number of shifts mapped to atoms	818
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

7.4.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	92	-0.49 ± 0.13	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\beta$	80	0.14 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

7.4.3 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 31%, i.e. 764 atoms were assigned a chemical shift out of a possible 2486. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	181/922 (20%)	96/380 (25%)	85/364 (23%)	0/178 (0%)
Sidechain	554/1420 (39%)	382/930 (41%)	172/434 (40%)	0/56 (0%)
Aromatic	29/144 (20%)	29/68 (43%)	0/68 (0%)	0/8 (0%)
Overall	764/2486 (31%)	507/1378 (37%)	257/866 (30%)	0/242 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 818 atoms were assigned a chemical shift out of a possible 2726. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	196/1004 (20%)	104/414 (25%)	92/396 (23%)	0/194 (0%)
Sidechain	591/1562 (38%)	408/1020 (40%)	183/474 (39%)	0/68 (0%)
Aromatic	31/160 (19%)	31/76 (41%)	0/72 (0%)	0/12 (0%)
Overall	818/2726 (30%)	543/1510 (36%)	275/942 (29%)	0/274 (0%)

7.4.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.4.5 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:

