



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 17, 2024 – 02:47 AM EDT

PDB ID : 5M1H  
BMRB ID : 34050  
Title : Structure of a Spumaretrovirus Gag central domain reveals an ancient retro-viral capsid  
Authors : Taylor, I.A.; Nicastro, G.; Ball, N.  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

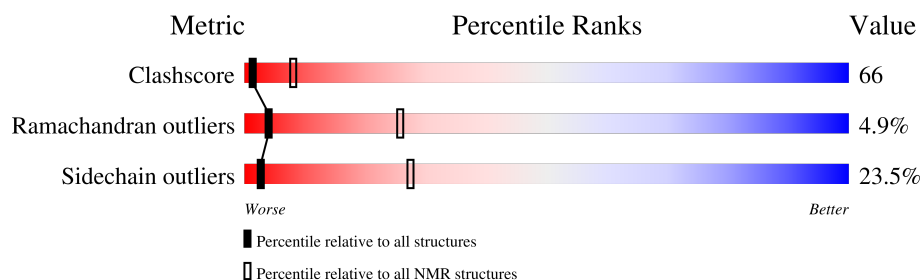
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

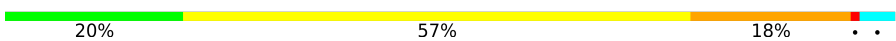
The overall completeness of chemical shifts assignment is 54%.

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  $\geq 3$ , 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	180	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:304-A:476 (173)	0.33	15

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2784 atoms, of which 1405 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gag protein.

Mol	Chain	Residues	Atoms						Trace
1	A	180	Total	C	H	N	O	S	0
			2784	872	1405	247	255	5	

There are 3 discrepancies between the modelled and reference sequences:

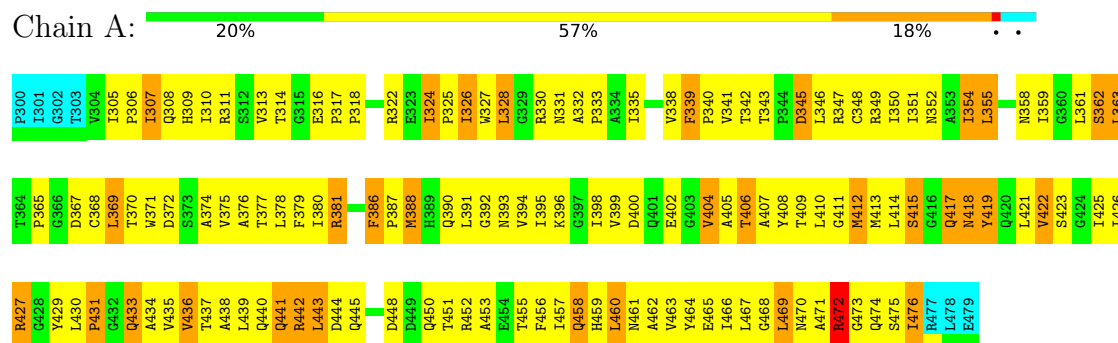
Chain	Residue	Modelled	Actual	Comment	Reference
A	449	ASP	ASN	engineered mutation	UNP P14349
A	478	LEU	-	expression tag	UNP P14349
A	479	GLU	-	expression tag	UNP P14349

## 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

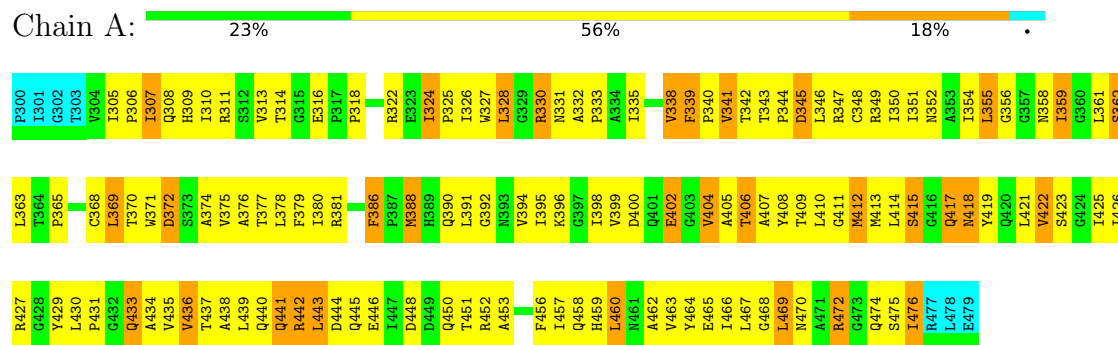


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

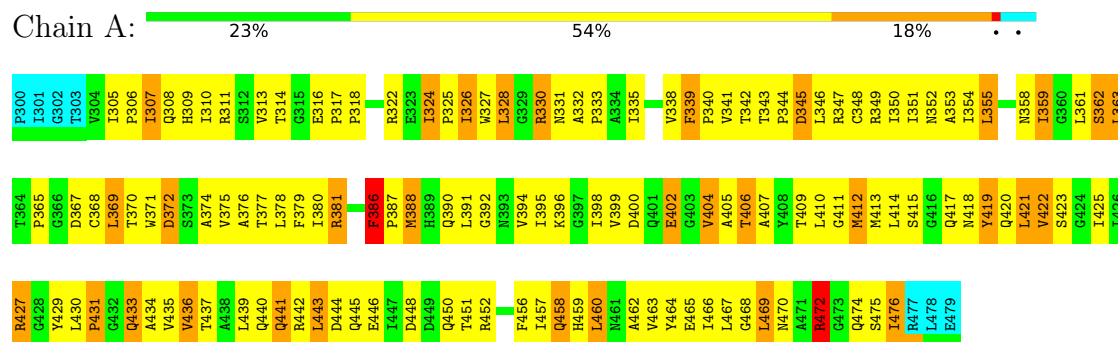
- Molecule 1: Gag protein





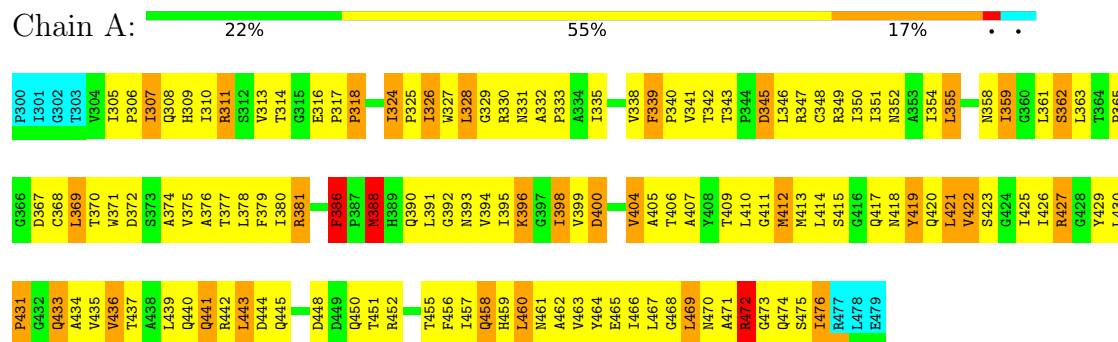
### 4.2.5 Score per residue for model 5

- Molecule 1: Gag protein



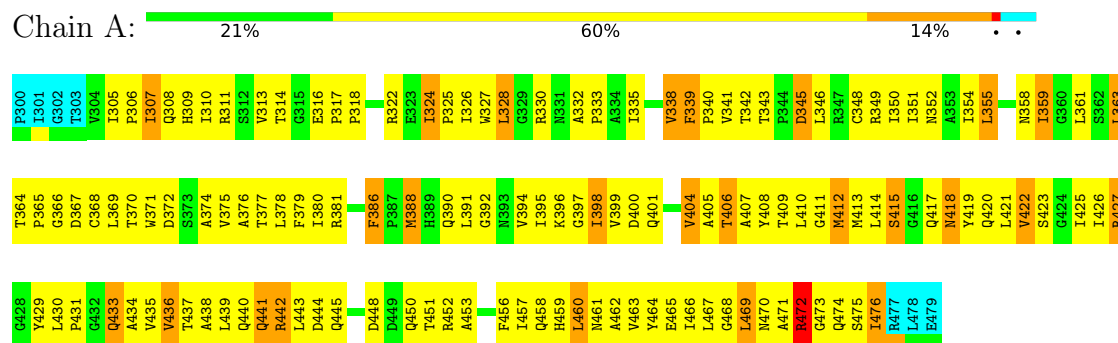
### 4.2.6 Score per residue for model 6

- Molecule 1: Gag protein



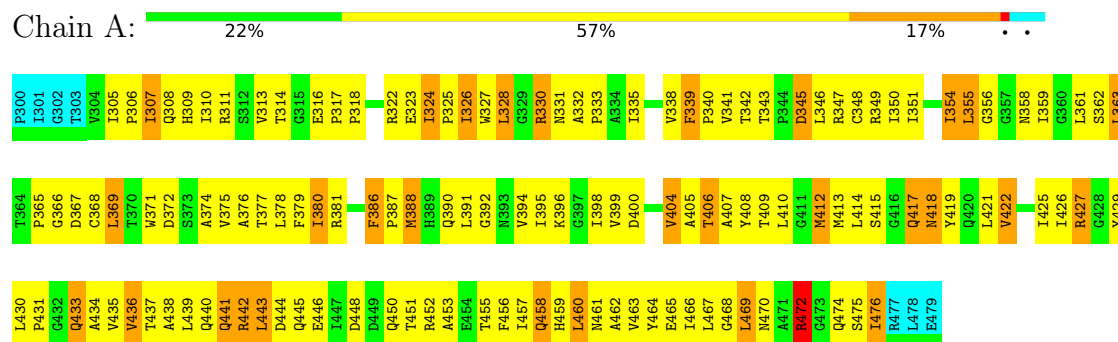
### 4.2.7 Score per residue for model 7

- Molecule 1: Gag protein



### 4.2.8 Score per residue for model 8

- Molecule 1: Gag protein



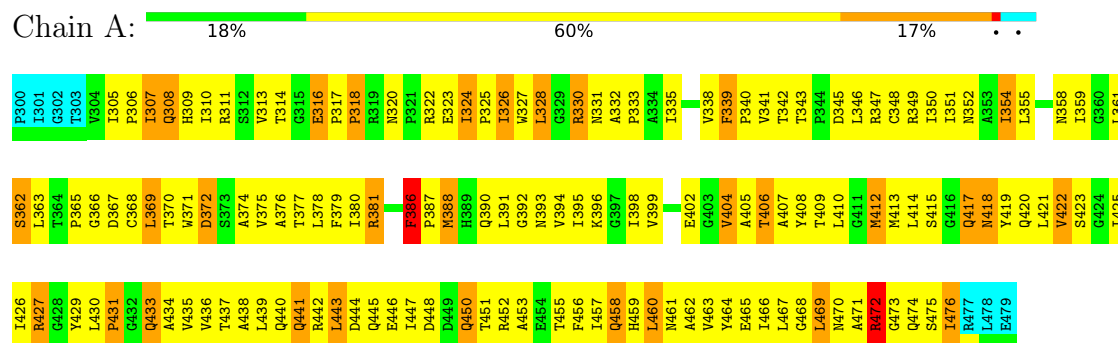
### 4.2.9 Score per residue for model 9

- Molecule 1: Gag protein



### 4.2.10 Score per residue for model 10

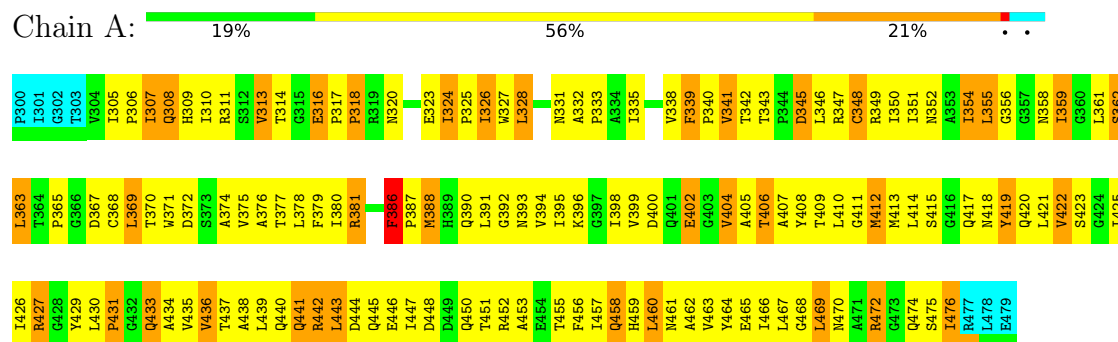
- Molecule 1: Gag protein





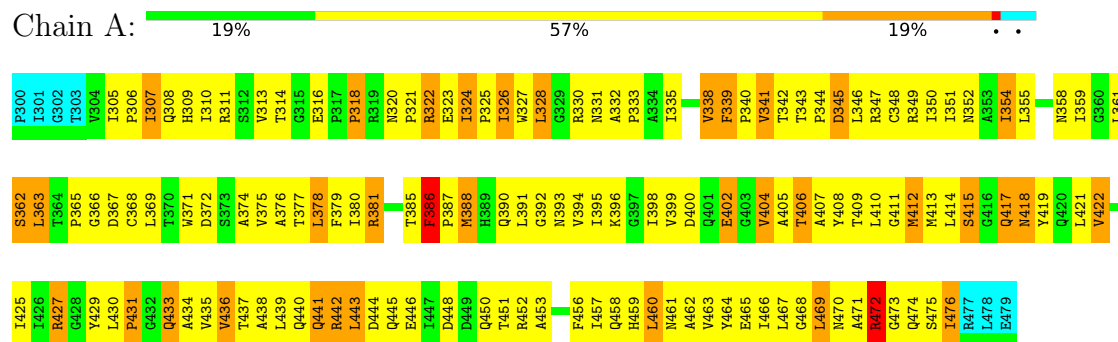
### 4.2.11 Score per residue for model 11

- Molecule 1: Gag protein



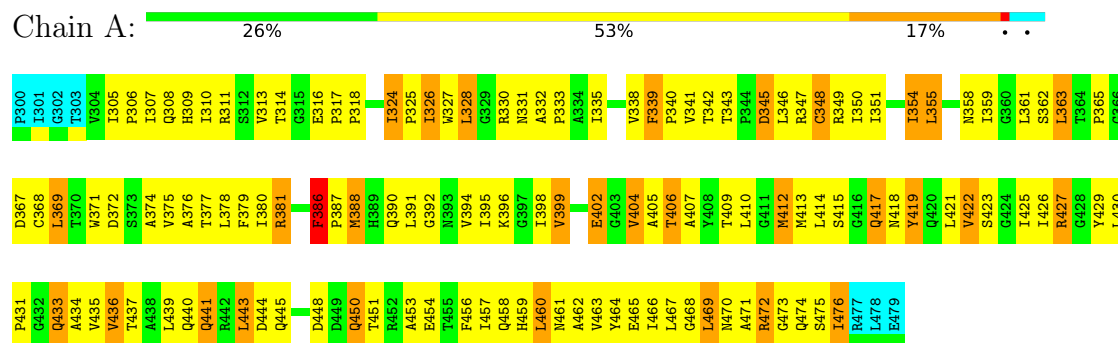
### 4.2.12 Score per residue for model 12

- Molecule 1: Gag protein



### 4.2.13 Score per residue for model 13

- Molecule 1: Gag protein



### 4.2.14 Score per residue for model 14

- Molecule 1: Gag protein



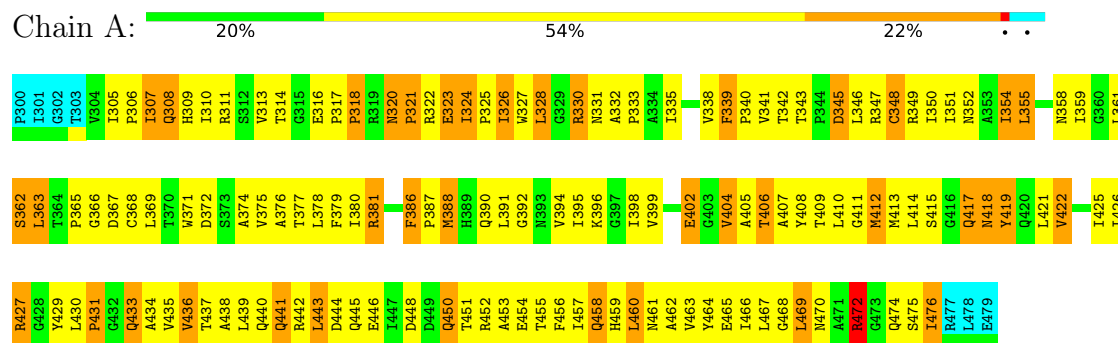
### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Gag protein



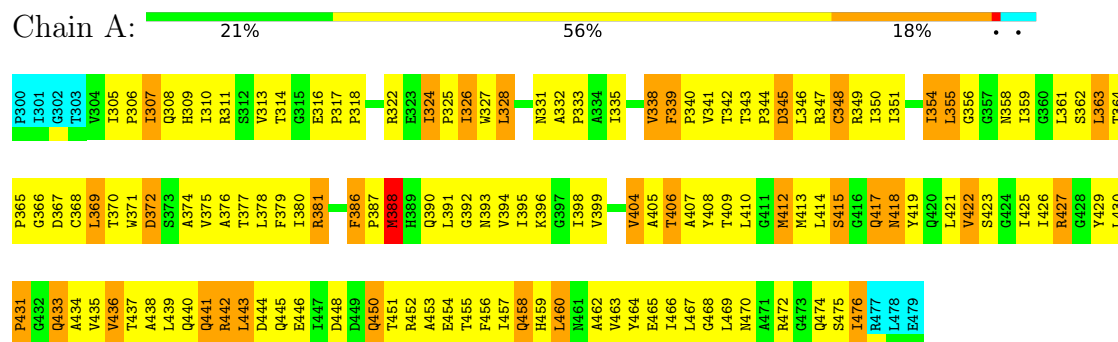
### 4.2.16 Score per residue for model 16

- Molecule 1: Gag protein



## 4.2.17 Score per residue for model 17

- Molecule 1: Gag protein



## 4.2.18 Score per residue for model 18

- Molecule 1: Gag protein



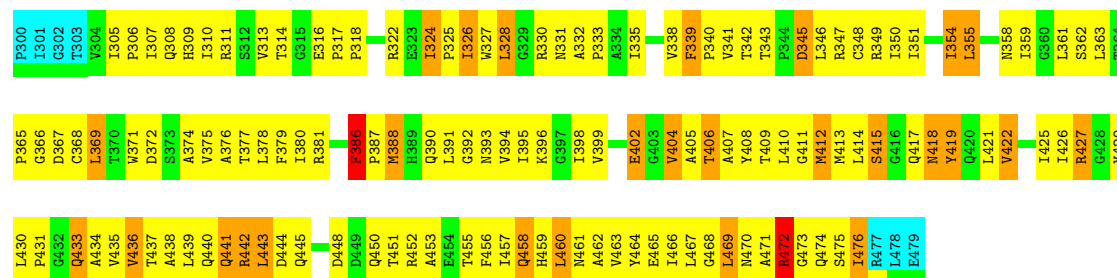
## 4.2.19 Score per residue for model 19

- Molecule 1: Gag protein



- Molecule 1: Gag protein

Frequency	Percentage
Daily	22%
Often	58%
Sometimes	15%
Never	4%



## 5 Refinement protocol and experimental data overview

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

Of the 100 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	1
Total number of shifts	1326
Number of shifts mapped to atoms	1326
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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	0.74±0.01	0±0/1351 ( 0.0± 0.0%)	0.85±0.01	1±0/1845 ( 0.1± 0.0%)
All	All	0.74	0/27020 ( 0.0%)	0.85	22/36900 ( 0.1%)

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	A	386	PHE	CB-CG-CD1	-7.19	115.77	120.80	17	20
1	A	339	PHE	CB-CG-CD1	-5.56	116.91	120.80	2	2

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1324	1345	1341	175±8
All	All	26480	26900	26820	3499

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 66.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:435:VAL:HA	1:A:463:VAL:HG11	1.05	1.29	6	20
1:A:348:CYS:SG	1:A:365:PRO:HA	1.00	1.96	1	13
1:A:348:CYS:SG	1:A:368:CYS:HB3	0.97	2.00	5	3
1:A:376:ALA:HA	1:A:414:LEU:HD23	0.93	1.38	7	20
1:A:348:CYS:SG	1:A:368:CYS:SG	0.88	2.72	17	14
1:A:419:TYR:HD2	1:A:423:SER:HG	0.86	1.05	17	1
1:A:391:LEU:HG	1:A:415:SER:OG	0.84	1.73	9	16
1:A:363:LEU:HB3	1:A:368:CYS:SG	0.81	2.15	18	9
1:A:348:CYS:SG	1:A:368:CYS:HB2	0.81	2.15	1	2
1:A:436:VAL:O	1:A:440:GLN:HG2	0.80	1.76	6	16
1:A:350:ILE:O	1:A:354:ILE:HG12	0.79	1.77	7	20
1:A:398:ILE:HB	1:A:407:ALA:HB2	0.78	1.55	3	20
1:A:318:PRO:HG3	1:A:327:TRP:CD1	0.77	2.15	11	9
1:A:339:PHE:CD2	1:A:350:ILE:HD11	0.77	2.13	17	18
1:A:439:LEU:O	1:A:443:LEU:HG	0.77	1.78	7	1
1:A:433:GLN:HA	1:A:436:VAL:HG13	0.77	1.56	3	20
1:A:439:LEU:O	1:A:443:LEU:HD22	0.76	1.81	12	19
1:A:314:THR:HB	1:A:327:TRP:CZ2	0.74	2.17	16	20
1:A:363:LEU:HD11	1:A:377:THR:HG21	0.74	1.60	8	18
1:A:399:VAL:HG12	1:A:404:VAL:HA	0.74	1.60	3	20
1:A:327:TRP:O	1:A:330:ARG:HB3	0.74	1.82	14	2
1:A:328:LEU:HB3	1:A:375:VAL:HG12	0.74	1.60	16	20
1:A:346:LEU:O	1:A:350:ILE:HG13	0.74	1.82	4	20
1:A:343:THR:OG1	1:A:346:LEU:HG	0.73	1.83	18	20
1:A:418:ASN:HD22	1:A:421:LEU:HD21	0.73	1.43	10	10
1:A:375:VAL:HG21	1:A:413:MET:HE3	0.73	1.59	20	19
1:A:418:ASN:ND2	1:A:421:LEU:HD23	0.73	1.99	11	2
1:A:409:THR:O	1:A:413:MET:HG3	0.72	1.84	7	20
1:A:318:PRO:HG2	1:A:323:GLU:OE1	0.72	1.84	11	1
1:A:305:ILE:HG12	1:A:339:PHE:CZ	0.72	2.18	4	20
1:A:421:LEU:HG	1:A:422:VAL:N	0.72	1.99	5	6
1:A:339:PHE:HD2	1:A:350:ILE:HD11	0.72	1.44	17	18
1:A:431:PRO:CB	1:A:472:ARG:HA	0.72	2.15	17	20
1:A:392:GLY:HA2	1:A:425:ILE:HD13	0.71	1.59	5	20
1:A:468:GLY:O	1:A:476:ILE:HG13	0.71	1.86	14	20
1:A:348:CYS:CB	1:A:368:CYS:HG	0.71	1.98	4	4
1:A:439:LEU:HD13	1:A:460:LEU:HD22	0.70	1.63	13	20
1:A:345:ASP:HA	1:A:348:CYS:SG	0.70	2.27	14	8
1:A:339:PHE:CD1	1:A:340:PRO:HD2	0.70	2.22	8	20
1:A:470:ASN:ND2	1:A:474:GLN:HG3	0.70	2.01	9	20
1:A:434:ALA:HB3	1:A:467:LEU:HD11	0.69	1.64	13	20
1:A:415:SER:HB3	1:A:418:ASN:ND2	0.69	2.02	1	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:418:ASN:HD22	1:A:421:LEU:HD23	0.69	1.47	11	2
1:A:443:LEU:HD23	1:A:444:ASP:N	0.68	2.02	4	19
1:A:395:ILE:O	1:A:399:VAL:HG22	0.68	1.88	13	20
1:A:418:ASN:ND2	1:A:421:LEU:HD21	0.68	2.04	16	15
1:A:358:ASN:ND2	1:A:361:LEU:HB2	0.67	2.04	13	17
1:A:440:GLN:O	1:A:444:ASP:HB2	0.67	1.90	2	20
1:A:307:ILE:O	1:A:311:ARG:HG3	0.66	1.90	4	20
1:A:463:VAL:HA	1:A:466:ILE:CD1	0.66	2.20	3	20
1:A:418:ASN:ND2	1:A:421:LEU:HD22	0.66	2.05	13	3
1:A:396:LYS:HD3	1:A:429:TYR:OH	0.65	1.91	17	17
1:A:439:LEU:CD1	1:A:460:LEU:HD22	0.65	2.22	3	20
1:A:398:ILE:HB	1:A:407:ALA:CB	0.65	2.22	4	20
1:A:439:LEU:HD21	1:A:460:LEU:HA	0.65	1.68	2	18
1:A:418:ASN:HD22	1:A:421:LEU:HD22	0.65	1.51	5	2
1:A:409:THR:HG22	1:A:413:MET:HE2	0.65	1.69	15	3
1:A:325:PRO:CB	1:A:379:PHE:HB2	0.65	2.21	14	20
1:A:427:ARG:HA	1:A:430:LEU:HD23	0.65	1.68	15	20
1:A:412:MET:HE2	1:A:417:GLN:HA	0.64	1.68	11	14
1:A:347:ARG:HA	1:A:350:ILE:HD12	0.64	1.68	5	15
1:A:418:ASN:O	1:A:421:LEU:HD23	0.64	1.93	5	3
1:A:399:VAL:HG21	1:A:429:TYR:CG	0.64	2.28	13	19
1:A:320:ASN:OD1	1:A:322:ARG:HG2	0.64	1.92	12	2
1:A:467:LEU:HD12	1:A:469:LEU:HD11	0.64	1.70	4	20
1:A:456:PHE:CE1	1:A:460:LEU:HD23	0.63	2.29	12	20
1:A:431:PRO:HB3	1:A:472:ARG:HA	0.63	1.68	4	20
1:A:392:GLY:O	1:A:396:LYS:HG2	0.63	1.92	7	16
1:A:422:VAL:HA	1:A:425:ILE:HD12	0.63	1.69	20	19
1:A:391:LEU:HG	1:A:415:SER:HG	0.63	1.52	16	6
1:A:324:ILE:HG12	1:A:355:LEU:HD11	0.63	1.70	2	8
1:A:374:ALA:O	1:A:378:LEU:HG	0.63	1.92	9	18
1:A:405:ALA:HA	1:A:457:ILE:HD12	0.63	1.71	10	20
1:A:365:PRO:HA	1:A:368:CYS:SG	0.63	2.34	14	5
1:A:324:ILE:HG12	1:A:355:LEU:CD1	0.63	2.24	1	16
1:A:468:GLY:O	1:A:475:SER:HA	0.63	1.94	19	20
1:A:433:GLN:HA	1:A:436:VAL:CG1	0.62	2.24	10	19
1:A:318:PRO:HG2	1:A:323:GLU:OE2	0.62	1.94	16	1
1:A:355:LEU:HD23	1:A:358:ASN:HD22	0.62	1.52	17	11
1:A:461:ASN:O	1:A:465:GLU:HG3	0.62	1.95	4	3
1:A:415:SER:OG	1:A:421:LEU:HD11	0.62	1.94	11	12
1:A:410:LEU:HD13	1:A:413:MET:CE	0.61	2.24	7	20
1:A:320:ASN:OD1	1:A:321:PRO:HD2	0.61	1.95	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:444:ASP:O	1:A:452:ARG:HD3	0.61	1.95	2	2
1:A:358:ASN:HD22	1:A:361:LEU:HB2	0.61	1.53	13	9
1:A:363:LEU:HD12	1:A:367:ASP:HB2	0.61	1.71	11	19
1:A:463:VAL:HA	1:A:466:ILE:CG1	0.60	2.26	3	20
1:A:365:PRO:HA	1:A:368:CYS:HG	0.60	1.56	14	3
1:A:324:ILE:N	1:A:325:PRO:HD2	0.60	2.12	7	20
1:A:463:VAL:HA	1:A:466:ILE:HG12	0.60	1.73	13	20
1:A:388:MET:HA	1:A:391:LEU:HD23	0.60	1.73	13	20
1:A:441:GLN:O	1:A:445:GLN:HG3	0.60	1.96	9	20
1:A:345:ASP:HA	1:A:365:PRO:CB	0.59	2.27	7	3
1:A:391:LEU:O	1:A:394:VAL:HG22	0.59	1.97	14	18
1:A:390:GLN:O	1:A:394:VAL:HG13	0.59	1.98	20	18
1:A:349:ARG:HA	1:A:352:ASN:OD1	0.59	1.97	3	1
1:A:394:VAL:O	1:A:398:ILE:HG13	0.59	1.98	6	12
1:A:371:TRP:O	1:A:375:VAL:HG13	0.59	1.98	18	20
1:A:326:ILE:HG21	1:A:398:ILE:HG12	0.59	1.75	10	14
1:A:327:TRP:CH2	1:A:354:ILE:HG21	0.59	2.33	6	17
1:A:348:CYS:SG	1:A:368:CYS:CB	0.58	2.91	1	4
1:A:419:TYR:CD1	1:A:453:ALA:HB2	0.58	2.34	18	12
1:A:408:TYR:OH	1:A:453:ALA:HA	0.58	1.99	18	16
1:A:363:LEU:HD12	1:A:367:ASP:CB	0.58	2.29	8	7
1:A:463:VAL:HA	1:A:466:ILE:HD11	0.58	1.75	3	20
1:A:412:MET:HE3	1:A:419:TYR:HB3	0.58	1.75	4	15
1:A:305:ILE:CD1	1:A:349:ARG:HB2	0.58	2.29	4	12
1:A:348:CYS:SG	1:A:365:PRO:CA	0.58	2.92	4	11
1:A:405:ALA:CA	1:A:457:ILE:HD12	0.57	2.29	10	20
1:A:435:VAL:HG12	1:A:439:LEU:CD1	0.57	2.29	5	20
1:A:361:LEU:HB3	1:A:378:LEU:HD22	0.57	1.75	17	17
1:A:452:ARG:O	1:A:456:PHE:HB2	0.57	1.99	2	19
1:A:345:ASP:O	1:A:349:ARG:HG3	0.57	1.98	14	19
1:A:347:ARG:HD2	1:A:368:CYS:O	0.57	1.99	17	11
1:A:359:ILE:HD12	1:A:359:ILE:N	0.57	2.14	17	20
1:A:342:THR:N	1:A:346:LEU:HD12	0.57	2.14	17	20
1:A:376:ALA:O	1:A:380:ILE:HD13	0.57	1.99	18	13
1:A:399:VAL:HG21	1:A:429:TYR:CD1	0.57	2.34	14	19
1:A:433:GLN:CA	1:A:436:VAL:HG13	0.57	2.28	10	5
1:A:317:PRO:HB3	1:A:324:ILE:HD11	0.57	1.75	8	12
1:A:359:ILE:HD12	1:A:359:ILE:H	0.57	1.59	2	15
1:A:461:ASN:O	1:A:465:GLU:HG2	0.57	2.00	10	10
1:A:447:ILE:HB	1:A:451:THR:HG21	0.57	1.75	2	4
1:A:314:THR:HG22	1:A:331:ASN:HB3	0.56	1.78	10	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:431:PRO:HB2	1:A:472:ARG:HA	0.56	1.76	17	9
1:A:376:ALA:HA	1:A:414:LEU:CD2	0.56	2.27	3	17
1:A:472:ARG:N	1:A:472:ARG:HD3	0.56	2.14	10	3
1:A:398:ILE:CG2	1:A:402:GLU:HG3	0.56	2.31	12	11
1:A:427:ARG:HD2	1:A:427:ARG:C	0.56	2.20	1	12
1:A:427:ARG:O	1:A:427:ARG:HD2	0.56	2.00	4	1
1:A:402:GLU:HG2	1:A:406:THR:CG2	0.56	2.31	3	2
1:A:339:PHE:CZ	1:A:346:LEU:HD13	0.56	2.36	17	19
1:A:418:ASN:ND2	1:A:421:LEU:CD2	0.56	2.69	3	5
1:A:307:ILE:HA	1:A:310:ILE:HD12	0.55	1.77	19	18
1:A:427:ARG:HA	1:A:430:LEU:CD2	0.55	2.30	9	18
1:A:326:ILE:O	1:A:330:ARG:HG3	0.55	2.02	2	1
1:A:330:ARG:HD3	1:A:402:GLU:OE1	0.55	2.02	12	1
1:A:435:VAL:HG13	1:A:463:VAL:HB	0.55	1.78	4	17
1:A:305:ILE:HG12	1:A:339:PHE:CE2	0.55	2.36	4	16
1:A:326:ILE:HA	1:A:410:LEU:HG	0.55	1.78	13	20
1:A:307:ILE:O	1:A:310:ILE:HB	0.55	2.02	9	16
1:A:310:ILE:HG23	1:A:335:ILE:HG23	0.54	1.79	6	20
1:A:307:ILE:HG23	1:A:308:GLN:N	0.54	2.18	9	17
1:A:351:ILE:O	1:A:355:LEU:HD22	0.54	2.01	4	8
1:A:305:ILE:HG22	1:A:307:ILE:H	0.54	1.63	19	10
1:A:406:THR:O	1:A:409:THR:HB	0.54	2.03	13	19
1:A:374:ALA:O	1:A:378:LEU:HD22	0.54	2.03	12	2
1:A:450:GLN:O	1:A:454:GLU:HG2	0.54	2.03	17	4
1:A:325:PRO:HA	1:A:378:LEU:HD23	0.54	1.80	2	2
1:A:435:VAL:HG12	1:A:439:LEU:HD12	0.54	1.78	5	3
1:A:398:ILE:HG23	1:A:402:GLU:HG3	0.54	1.78	12	5
1:A:372:ASP:HA	1:A:413:MET:SD	0.54	2.43	7	19
1:A:411:GLY:O	1:A:415:SER:HB2	0.54	2.03	15	7
1:A:448:ASP:O	1:A:452:ARG:HG3	0.54	2.03	7	9
1:A:328:LEU:HD23	1:A:331:ASN:OD1	0.54	2.03	15	3
1:A:306:PRO:HD2	1:A:339:PHE:CD1	0.54	2.38	13	5
1:A:307:ILE:HG23	1:A:308:GLN:H	0.54	1.63	19	15
1:A:412:MET:CE	1:A:417:GLN:HA	0.54	2.33	10	19
1:A:306:PRO:O	1:A:308:GLN:N	0.54	2.41	17	15
1:A:363:LEU:HD21	1:A:377:THR:CG2	0.54	2.33	12	10
1:A:378:LEU:O	1:A:381:ARG:HB2	0.53	2.02	13	20
1:A:410:LEU:O	1:A:414:LEU:HG	0.53	2.03	18	19
1:A:459:HIS:O	1:A:463:VAL:HG23	0.53	2.03	12	20
1:A:427:ARG:C	1:A:427:ARG:HD3	0.53	2.24	10	2
1:A:363:LEU:HD23	1:A:378:LEU:CD1	0.53	2.33	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:355:LEU:HD23	1:A:358:ASN:ND2	0.53	2.19	13	7
1:A:368:CYS:SG	1:A:368:CYS:O	0.53	2.67	3	2
1:A:402:GLU:HG2	1:A:406:THR:HG21	0.53	1.79	3	2
1:A:354:ILE:HB	1:A:355:LEU:HD13	0.53	1.80	5	18
1:A:398:ILE:CD1	1:A:407:ALA:HA	0.53	2.33	3	8
1:A:435:VAL:CA	1:A:463:VAL:HG11	0.53	2.20	14	16
1:A:464:TYR:O	1:A:469:LEU:N	0.53	2.42	2	20
1:A:345:ASP:CA	1:A:348:CYS:SG	0.53	2.97	11	7
1:A:309:HIS:CD2	1:A:338:VAL:HG22	0.53	2.39	3	20
1:A:330:ARG:NH1	1:A:402:GLU:HB2	0.53	2.18	10	1
1:A:307:ILE:HG23	1:A:308:GLN:HG2	0.53	1.81	5	7
1:A:434:ALA:HB3	1:A:467:LEU:CD1	0.53	2.34	16	13
1:A:344:PRO:HB3	1:A:369:LEU:HD12	0.53	1.80	1	3
1:A:363:LEU:HD23	1:A:378:LEU:HD23	0.53	1.81	1	12
1:A:405:ALA:HA	1:A:457:ILE:CD1	0.52	2.34	16	20
1:A:439:LEU:HB3	1:A:443:LEU:HD13	0.52	1.81	16	16
1:A:439:LEU:HB3	1:A:443:LEU:HD21	0.52	1.81	7	1
1:A:439:LEU:HG	1:A:463:VAL:HG21	0.52	1.81	13	18
1:A:324:ILE:O	1:A:327:TRP:HB3	0.52	2.04	10	17
1:A:332:ALA:HA	1:A:335:ILE:HD12	0.52	1.82	7	12
1:A:412:MET:HE1	1:A:419:TYR:HB3	0.52	1.80	1	3
1:A:472:ARG:HB2	1:A:474:GLN:HE21	0.52	1.65	17	1
1:A:443:LEU:HD22	1:A:456:PHE:CD2	0.52	2.39	7	1
1:A:415:SER:HB3	1:A:418:ASN:HD21	0.52	1.63	3	6
1:A:399:VAL:HG12	1:A:404:VAL:CA	0.52	2.34	10	1
1:A:359:ILE:H	1:A:359:ILE:CD1	0.52	2.18	2	18
1:A:320:ASN:HB2	1:A:323:GLU:HG3	0.52	1.82	16	1
1:A:328:LEU:HD11	1:A:351:ILE:HG12	0.52	1.82	3	8
1:A:324:ILE:HG21	1:A:355:LEU:HD21	0.52	1.81	12	11
1:A:339:PHE:CD2	1:A:341:VAL:HG22	0.52	2.40	4	1
1:A:310:ILE:HG21	1:A:350:ILE:CG2	0.52	2.35	15	13
1:A:462:ALA:O	1:A:465:GLU:HB2	0.51	2.05	16	13
1:A:402:GLU:HG2	1:A:406:THR:CB	0.51	2.36	3	2
1:A:463:VAL:HG13	1:A:466:ILE:HD11	0.51	1.83	6	15
1:A:320:ASN:H	1:A:323:GLU:CG	0.51	2.17	11	1
1:A:320:ASN:H	1:A:323:GLU:HG2	0.51	1.66	10	2
1:A:462:ALA:O	1:A:465:GLU:HB3	0.51	2.06	2	6
1:A:455:THR:HB	1:A:458:GLN:NE2	0.51	2.20	20	13
1:A:358:ASN:HB2	1:A:361:LEU:HD12	0.51	1.82	13	3
1:A:418:ASN:HD21	1:A:421:LEU:HD21	0.50	1.65	3	4
1:A:388:MET:SD	1:A:421:LEU:CD1	0.50	2.99	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:324:ILE:HA	1:A:327:TRP:HB3	0.50	1.84	16	9
1:A:352:ASN:OD1	1:A:362:SER:HA	0.50	2.06	4	11
1:A:320:ASN:HB3	1:A:321:PRO:HD2	0.50	1.82	16	1
1:A:436:VAL:CG2	1:A:437:THR:N	0.50	2.74	6	18
1:A:321:PRO:O	1:A:324:ILE:HB	0.50	2.07	14	3
1:A:419:TYR:O	1:A:422:VAL:HG22	0.50	2.06	19	12
1:A:328:LEU:HD12	1:A:378:LEU:HD11	0.50	1.83	14	8
1:A:348:CYS:HA	1:A:368:CYS:SG	0.50	2.46	3	3
1:A:394:VAL:HG11	1:A:414:LEU:CD1	0.50	2.37	7	2
1:A:327:TRP:O	1:A:330:ARG:HG3	0.50	2.07	4	3
1:A:320:ASN:HB2	1:A:323:GLU:CG	0.50	2.37	16	2
1:A:325:PRO:HA	1:A:378:LEU:HD12	0.49	1.84	19	8
1:A:415:SER:HB2	1:A:421:LEU:HD21	0.49	1.83	6	1
1:A:396:LYS:HD2	1:A:429:TYR:OH	0.49	2.07	8	1
1:A:308:GLN:HA	1:A:308:GLN:OE1	0.49	2.07	3	1
1:A:363:LEU:HD23	1:A:378:LEU:CD2	0.49	2.36	6	12
1:A:459:HIS:O	1:A:462:ALA:HB3	0.49	2.07	20	14
1:A:399:VAL:HG11	1:A:429:TYR:CB	0.49	2.38	13	2
1:A:330:ARG:HD2	1:A:406:THR:HG21	0.49	1.85	5	6
1:A:443:LEU:HD12	1:A:444:ASP:N	0.49	2.22	7	1
1:A:339:PHE:CE2	1:A:350:ILE:HD11	0.49	2.42	20	4
1:A:368:CYS:O	1:A:368:CYS:SG	0.49	2.71	12	1
1:A:352:ASN:CG	1:A:362:SER:HA	0.49	2.28	12	13
1:A:305:ILE:HG22	1:A:307:ILE:N	0.49	2.23	18	2
1:A:361:LEU:HB3	1:A:378:LEU:HD12	0.49	1.85	12	2
1:A:309:HIS:CG	1:A:338:VAL:HG13	0.49	2.43	11	15
1:A:339:PHE:CE2	1:A:346:LEU:HB3	0.49	2.43	13	16
1:A:307:ILE:HG12	1:A:353:ALA:HB1	0.49	1.85	4	3
1:A:386:PHE:CE2	1:A:391:LEU:HD21	0.49	2.43	11	9
1:A:398:ILE:HG21	1:A:406:THR:HG22	0.49	1.85	10	1
1:A:310:ILE:HG13	1:A:338:VAL:HG11	0.48	1.84	19	19
1:A:326:ILE:HG13	1:A:410:LEU:HG	0.48	1.84	19	20
1:A:430:LEU:HD22	1:A:430:LEU:N	0.48	2.23	2	19
1:A:348:CYS:CB	1:A:368:CYS:SG	0.48	3.01	10	10
1:A:345:ASP:HA	1:A:365:PRO:HB3	0.48	1.86	1	10
1:A:393:ASN:HA	1:A:396:LYS:HG3	0.48	1.84	18	10
1:A:310:ILE:CG2	1:A:335:ILE:HG23	0.48	2.39	5	20
1:A:388:MET:CE	1:A:415:SER:HA	0.48	2.38	1	5
1:A:406:THR:O	1:A:410:LEU:HD22	0.48	2.07	14	15
1:A:388:MET:SD	1:A:421:LEU:HD11	0.48	2.48	5	1
1:A:332:ALA:N	1:A:333:PRO:HD2	0.48	2.24	14	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:457:ILE:HA	1:A:460:LEU:HB2	0.48	1.84	7	19
1:A:423:SER:HG	1:A:456:PHE:HE2	0.48	1.51	14	4
1:A:439:LEU:HD21	1:A:460:LEU:CA	0.48	2.39	2	10
1:A:330:ARG:HD3	1:A:406:THR:HG21	0.48	1.86	10	1
1:A:363:LEU:CB	1:A:368:CYS:SG	0.48	3.02	2	3
1:A:431:PRO:HB2	1:A:473:GLY:N	0.47	2.23	4	2
1:A:421:LEU:HG	1:A:422:VAL:H	0.47	1.69	18	8
1:A:415:SER:CB	1:A:421:LEU:HD21	0.47	2.39	13	2
1:A:438:ALA:O	1:A:442:ARG:HG2	0.47	2.09	16	2
1:A:366:GLY:O	1:A:369:LEU:HD11	0.47	2.09	10	6
1:A:446:GLU:HB2	1:A:452:ARG:CG	0.47	2.38	5	7
1:A:310:ILE:O	1:A:314:THR:HG23	0.47	2.10	2	14
1:A:361:LEU:HB3	1:A:378:LEU:HB3	0.47	1.86	3	6
1:A:474:GLN:O	1:A:475:SER:HB3	0.47	2.10	10	6
1:A:336:ASP:HA	1:A:339:PHE:O	0.47	2.10	4	1
1:A:427:ARG:CA	1:A:430:LEU:HD23	0.47	2.40	20	12
1:A:410:LEU:HA	1:A:413:MET:HE2	0.47	1.87	3	7
1:A:317:PRO:HG3	1:A:355:LEU:HD12	0.47	1.86	7	4
1:A:435:VAL:HG12	1:A:439:LEU:HD11	0.47	1.86	4	14
1:A:313:VAL:HG12	1:A:314:THR:HG23	0.47	1.85	11	3
1:A:398:ILE:HG22	1:A:402:GLU:HG3	0.46	1.87	2	3
1:A:399:VAL:HG21	1:A:429:TYR:CE1	0.46	2.45	3	2
1:A:419:TYR:CD2	1:A:419:TYR:C	0.46	2.89	6	9
1:A:307:ILE:HD13	1:A:350:ILE:HA	0.46	1.86	20	5
1:A:405:ALA:HB1	1:A:457:ILE:HG23	0.46	1.85	10	11
1:A:395:ILE:HG23	1:A:426:ILE:HD13	0.46	1.87	8	11
1:A:404:VAL:HG13	1:A:464:TYR:OH	0.46	2.10	5	9
1:A:310:ILE:HG23	1:A:335:ILE:HG12	0.46	1.87	7	14
1:A:397:GLY:O	1:A:401:GLN:HG3	0.46	2.09	15	2
1:A:339:PHE:CD2	1:A:341:VAL:HB	0.46	2.45	12	2
1:A:448:ASP:H	1:A:451:THR:HB	0.46	1.70	4	20
1:A:391:LEU:O	1:A:394:VAL:HB	0.46	2.11	3	1
1:A:318:PRO:HG2	1:A:323:GLU:CD	0.46	2.31	11	1
1:A:344:PRO:HB3	1:A:369:LEU:HD23	0.46	1.87	12	1
1:A:375:VAL:HA	1:A:378:LEU:CD2	0.46	2.40	2	1
1:A:436:VAL:O	1:A:440:GLN:HB2	0.46	2.11	2	3
1:A:376:ALA:CA	1:A:414:LEU:HD23	0.46	2.32	16	7
1:A:411:GLY:HA2	1:A:414:LEU:HD12	0.46	1.87	12	9
1:A:392:GLY:O	1:A:396:LYS:HG3	0.46	2.10	8	1
1:A:390:GLN:O	1:A:394:VAL:HG23	0.46	2.11	7	2
1:A:369:LEU:HD13	1:A:369:LEU:N	0.46	2.25	17	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:366:GLY:HA2	1:A:369:LEU:HD21	0.46	1.87	12	1
1:A:376:ALA:CB	1:A:414:LEU:HA	0.46	2.41	2	4
1:A:342:THR:H	1:A:346:LEU:HD12	0.46	1.71	10	9
1:A:418:ASN:HD22	1:A:421:LEU:CD2	0.46	2.24	17	6
1:A:363:LEU:HD21	1:A:377:THR:HG22	0.45	1.87	4	5
1:A:419:TYR:HD2	1:A:423:SER:OG	0.45	1.94	13	1
1:A:355:LEU:HG	1:A:358:ASN:HD22	0.45	1.71	15	1
1:A:439:LEU:HD21	1:A:459:HIS:O	0.45	2.12	3	2
1:A:344:PRO:O	1:A:347:ARG:HB2	0.45	2.12	4	1
1:A:420:GLN:O	1:A:423:SER:HB3	0.45	2.11	10	9
1:A:341:VAL:HG23	1:A:346:LEU:CB	0.45	2.41	12	1
1:A:415:SER:HG	1:A:421:LEU:HD11	0.45	1.72	13	2
1:A:423:SER:HA	1:A:426:ILE:HB	0.45	1.88	17	3
1:A:472:ARG:N	1:A:472:ARG:CD	0.45	2.80	14	8
1:A:375:VAL:HG21	1:A:413:MET:CE	0.45	2.41	18	1
1:A:377:THR:HA	1:A:380:ILE:HB	0.45	1.88	12	13
1:A:325:PRO:HB2	1:A:379:PHE:HB2	0.45	1.89	14	15
1:A:328:LEU:HD11	1:A:351:ILE:HG23	0.45	1.88	13	6
1:A:471:ALA:O	1:A:473:GLY:N	0.45	2.50	19	12
1:A:345:ASP:OD1	1:A:349:ARG:HD2	0.45	2.11	7	1
1:A:433:GLN:NE2	1:A:437:THR:OG1	0.45	2.49	10	1
1:A:421:LEU:CG	1:A:422:VAL:N	0.45	2.79	13	1
1:A:459:HIS:HA	1:A:462:ALA:HB3	0.45	1.89	18	9
1:A:464:TYR:CZ	1:A:471:ALA:HA	0.45	2.47	19	1
1:A:351:ILE:HD13	1:A:374:ALA:HB1	0.44	1.89	16	11
1:A:316:GLU:HB3	1:A:317:PRO:HD2	0.44	1.89	9	3
1:A:392:GLY:O	1:A:396:LYS:HB2	0.44	2.11	19	1
1:A:394:VAL:HG11	1:A:414:LEU:HD13	0.44	1.87	3	1
1:A:327:TRP:HH2	1:A:354:ILE:HG21	0.44	1.71	14	2
1:A:346:LEU:O	1:A:350:ILE:CG1	0.44	2.65	6	2
1:A:364:THR:C	1:A:366:GLY:H	0.44	2.14	17	3
1:A:358:ASN:HB2	1:A:361:LEU:HG	0.44	1.90	20	8
1:A:391:LEU:O	1:A:395:ILE:HG12	0.44	2.13	20	1
1:A:399:VAL:HG23	1:A:400:ASP:N	0.44	2.28	1	13
1:A:317:PRO:HG3	1:A:355:LEU:HA	0.44	1.90	11	1
1:A:348:CYS:HB3	1:A:368:CYS:HG	0.44	1.72	16	1
1:A:412:MET:HE3	1:A:417:GLN:HA	0.43	1.90	1	3
1:A:326:ILE:CA	1:A:410:LEU:HG	0.43	2.42	13	5
1:A:423:SER:O	1:A:427:ARG:HB3	0.43	2.13	6	1
1:A:359:ILE:N	1:A:359:ILE:CD1	0.43	2.81	13	3
1:A:402:GLU:HG2	1:A:406:THR:HB	0.43	1.89	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:348:CYS:HB2	1:A:368:CYS:SG	0.43	2.52	6	1
1:A:450:GLN:HA	1:A:453:ALA:HB3	0.43	1.90	10	3
1:A:326:ILE:CG1	1:A:410:LEU:HG	0.43	2.43	16	10
1:A:398:ILE:HD12	1:A:407:ALA:HA	0.43	1.89	3	1
1:A:463:VAL:O	1:A:467:LEU:HG	0.43	2.13	3	1
1:A:344:PRO:O	1:A:348:CYS:SG	0.43	2.75	4	2
1:A:388:MET:SD	1:A:391:LEU:HD23	0.43	2.54	5	1
1:A:404:VAL:HG23	1:A:426:ILE:HG23	0.43	1.89	9	8
1:A:326:ILE:CG2	1:A:398:ILE:HG12	0.43	2.44	13	1
1:A:324:ILE:HD13	1:A:358:ASN:HD21	0.43	1.73	15	1
1:A:329:GLY:HA3	1:A:410:LEU:CD1	0.43	2.43	4	2
1:A:326:ILE:HA	1:A:410:LEU:CD1	0.43	2.44	8	6
1:A:348:CYS:HB3	1:A:368:CYS:SG	0.43	2.53	16	2
1:A:377:THR:O	1:A:381:ARG:HD3	0.43	2.14	19	6
1:A:341:VAL:HG21	1:A:347:ARG:HG3	0.43	1.91	11	1
1:A:320:ASN:HB3	1:A:323:GLU:HG3	0.43	1.89	12	2
1:A:438:ALA:O	1:A:442:ARG:CG	0.43	2.67	12	14
1:A:324:ILE:HD13	1:A:358:ASN:ND2	0.43	2.28	15	1
1:A:355:LEU:HG	1:A:358:ASN:ND2	0.43	2.28	15	1
1:A:421:LEU:HD12	1:A:422:VAL:N	0.42	2.29	11	2
1:A:314:THR:HB	1:A:327:TRP:CH2	0.42	2.49	16	2
1:A:456:PHE:O	1:A:460:LEU:HB2	0.42	2.15	9	5
1:A:363:LEU:HD13	1:A:363:LEU:HA	0.42	1.72	14	2
1:A:443:LEU:HD23	1:A:443:LEU:C	0.42	2.34	15	12
1:A:388:MET:HE1	1:A:415:SER:HA	0.42	1.90	5	1
1:A:341:VAL:HG21	1:A:347:ARG:HG2	0.42	1.90	12	1
1:A:405:ALA:CB	1:A:457:ILE:HD12	0.42	2.44	2	2
1:A:438:ALA:O	1:A:441:GLN:HB2	0.42	2.15	7	1
1:A:327:TRP:HA	1:A:330:ARG:HG3	0.42	1.90	10	1
1:A:325:PRO:HB3	1:A:379:PHE:N	0.42	2.29	16	1
1:A:386:PHE:HB3	1:A:390:GLN:HB2	0.42	1.91	20	1
1:A:307:ILE:CG2	1:A:308:GLN:N	0.42	2.83	5	2
1:A:379:PHE:CD1	1:A:414:LEU:HD22	0.42	2.49	14	2
1:A:409:THR:HG22	1:A:413:MET:CE	0.42	2.45	14	2
1:A:396:LYS:HG3	1:A:429:TYR:OH	0.42	2.14	6	1
1:A:430:LEU:CB	1:A:436:VAL:HG12	0.42	2.44	6	3
1:A:411:GLY:O	1:A:415:SER:HB3	0.42	2.13	14	1
1:A:375:VAL:HG23	1:A:376:ALA:N	0.42	2.30	4	10
1:A:443:LEU:O	1:A:452:ARG:HG2	0.42	2.15	2	1
1:A:310:ILE:HD11	1:A:339:PHE:HB2	0.42	1.92	10	8
1:A:399:VAL:HG21	1:A:429:TYR:CD2	0.42	2.50	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:459:HIS:HA	1:A:462:ALA:CB	0.42	2.45	18	1
1:A:330:ARG:CD	1:A:406:THR:HG21	0.41	2.45	16	2
1:A:330:ARG:HD3	1:A:402:GLU:OE2	0.41	2.15	13	1
1:A:410:LEU:HD22	1:A:410:LEU:H	0.41	1.76	1	1
1:A:457:ILE:HA	1:A:460:LEU:CB	0.41	2.45	16	8
1:A:324:ILE:HG12	1:A:355:LEU:HG	0.41	1.92	13	1
1:A:361:LEU:O	1:A:363:LEU:N	0.41	2.53	13	1
1:A:419:TYR:CZ	1:A:420:GLN:HG2	0.41	2.51	15	1
1:A:446:GLU:HB3	1:A:451:THR:CG2	0.41	2.46	16	4
1:A:359:ILE:CD1	1:A:359:ILE:N	0.41	2.84	3	4
1:A:372:ASP:OD2	1:A:413:MET:HG2	0.41	2.15	7	1
1:A:404:VAL:HG11	1:A:430:LEU:HD13	0.41	1.92	14	2
1:A:417:GLN:N	1:A:417:GLN:CD	0.41	2.74	13	1
1:A:350:ILE:O	1:A:354:ILE:CG1	0.41	2.68	18	2
1:A:363:LEU:CD2	1:A:378:LEU:HD23	0.41	2.45	6	1
1:A:339:PHE:HD2	1:A:350:ILE:CD1	0.41	2.28	7	2
1:A:398:ILE:CG2	1:A:406:THR:HG22	0.41	2.46	10	1
1:A:430:LEU:CD2	1:A:430:LEU:N	0.41	2.83	2	9
1:A:435:VAL:O	1:A:439:LEU:HB2	0.41	2.15	5	1
1:A:458:GLN:HG2	1:A:459:HIS:N	0.41	2.31	5	2
1:A:324:ILE:HG12	1:A:355:LEU:CG	0.41	2.45	13	1
1:A:341:VAL:HG22	1:A:341:VAL:O	0.41	2.16	3	2
1:A:430:LEU:N	1:A:430:LEU:CD2	0.41	2.84	1	2
1:A:313:VAL:HG12	1:A:314:THR:N	0.41	2.31	9	3
1:A:440:GLN:NE2	1:A:440:GLN:HA	0.41	2.30	6	1
1:A:375:VAL:CG2	1:A:376:ALA:N	0.41	2.84	8	4
1:A:316:GLU:HB3	1:A:317:PRO:CD	0.41	2.46	11	2
1:A:358:ASN:HB2	1:A:361:LEU:CD1	0.41	2.46	13	1
1:A:308:GLN:HA	1:A:311:ARG:HD3	0.41	1.93	20	1
1:A:427:ARG:O	1:A:430:LEU:HD23	0.41	2.16	1	2
1:A:456:PHE:HE1	1:A:460:LEU:HD23	0.41	1.71	3	1
1:A:359:ILE:CD1	1:A:359:ILE:H	0.41	2.29	13	1
1:A:355:LEU:CD2	1:A:358:ASN:HD22	0.41	2.24	17	1
1:A:427:ARG:C	1:A:427:ARG:HD2	0.40	2.36	5	2
1:A:343:THR:HG1	1:A:346:LEU:HG	0.40	1.74	2	1
1:A:361:LEU:HB3	1:A:378:LEU:CD2	0.40	2.45	13	1
1:A:393:ASN:HA	1:A:396:LYS:HE3	0.40	1.92	6	1
1:A:314:THR:CB	1:A:327:TRP:CZ2	0.40	3.02	15	1
1:A:314:THR:HA	1:A:331:ASN:CG	0.40	2.36	16	1
1:A:345:ASP:O	1:A:348:CYS:SG	0.40	2.79	16	1
1:A:412:MET:CE	1:A:419:TYR:HB3	0.40	2.47	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:439:LEU:O	1:A:443:LEU:CG	0.40	2.62	7	1
1:A:398:ILE:HD13	1:A:407:ALA:HA	0.40	1.94	10	1
1:A:361:LEU:O	1:A:378:LEU:HD12	0.40	2.16	12	1
1:A:306:PRO:CD	1:A:339:PHE:CD1	0.40	3.04	13	1
1:A:325:PRO:O	1:A:375:VAL:HB	0.40	2.17	16	1
1:A:325:PRO:HB3	1:A:375:VAL:O	0.40	2.16	2	1
1:A:450:GLN:HA	1:A:453:ALA:CB	0.40	2.47	9	1
1:A:318:PRO:HB3	1:A:327:TRP:CD1	0.40	2.52	12	1
1:A:464:TYR:HD1	1:A:469:LEU:HD12	0.40	1.76	19	1
1:A:458:GLN:O	1:A:462:ALA:HB2	0.40	2.17	20	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	173/180 (96%)	149±2 (86±1%)	15±2 (9±1%)	9±1 (5±1%)	4	26
All	All	3460/3600 (96%)	2987 (86%)	302 (9%)	171 (5%)	4	26

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	316	GLU	20
1	A	318	PRO	20
1	A	341	VAL	19
1	A	362	SER	18
1	A	472	ARG	18
1	A	307	ILE	15
1	A	387	PRO	14
1	A	431	PRO	13
1	A	359	ILE	8
1	A	338	VAL	7
1	A	356	GLY	6
1	A	363	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	388	MET	4
1	A	357	GLY	1
1	A	471	ALA	1
1	A	365	PRO	1
1	A	320	ASN	1
1	A	321	PRO	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	143/149 (96%)	109±2 (77±1%)	34±2 (23±1%)	3	27
All	All	2860/2980 (96%)	2189 (77%)	671 (23%)	3	27

All 52 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	313	VAL	20
1	A	324	ILE	20
1	A	328	LEU	20
1	A	339	PHE	20
1	A	386	PHE	20
1	A	404	VAL	20
1	A	412	MET	20
1	A	422	VAL	20
1	A	433	GLN	20
1	A	441	GLN	20
1	A	450	GLN	20
1	A	458	GLN	20
1	A	460	LEU	20
1	A	476	ILE	20
1	A	436	VAL	19
1	A	443	LEU	19
1	A	469	LEU	19
1	A	345	ASP	18
1	A	355	LEU	18

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Mol	Chain	Res	Type	Models (Total)
1	A	388	MET	18
1	A	406	THR	18
1	A	427	ARG	18
1	A	369	LEU	17
1	A	326	ILE	17
1	A	442	ARG	16
1	A	322	ARG	15
1	A	418	ASN	15
1	A	472	ARG	15
1	A	370	THR	13
1	A	381	ARG	13
1	A	354	ILE	13
1	A	402	GLU	11
1	A	417	GLN	11
1	A	419	TYR	11
1	A	415	SER	10
1	A	363	LEU	10
1	A	308	GLN	9
1	A	330	ARG	8
1	A	348	CYS	8
1	A	372	ASP	7
1	A	380	ILE	7
1	A	398	ILE	3
1	A	378	LEU	2
1	A	352	ASN	2
1	A	421	LEU	2
1	A	396	LYS	2
1	A	323	GLU	2
1	A	311	ARG	1
1	A	400	ASP	1
1	A	385	THR	1
1	A	399	VAL	1
1	A	331	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 monosaccharides 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 54% for the well-defined parts and 54% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: 15N-HPFV-300-477-11052015-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	1326
Number of shifts mapped to atoms	1326
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	164	$0.83 \pm 0.26$	Should be applied

#### 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 54%, i.e. 1286 atoms were assigned a chemical shift out of a possible 2363. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	487/861 (57%)	328/353 (93%)	0/346 (0%)	159/162 (98%)
Sidechain	776/1370 (57%)	757/900 (84%)	0/416 (0%)	19/54 (35%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	23/132 (17%)	23/64 (36%)	0/58 (0%)	0/10 (0%)
Overall	1286/2363 (54%)	1108/1317 (84%)	0/820 (0%)	178/226 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 54%, i.e. 1325 atoms were assigned a chemical shift out of a possible 2463. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	504/895 (56%)	340/367 (93%)	0/360 (0%)	164/168 (98%)
Sidechain	798/1436 (56%)	779/943 (83%)	0/436 (0%)	19/57 (33%)
Aromatic	23/132 (17%)	23/64 (36%)	0/58 (0%)	0/10 (0%)
Overall	1325/2463 (54%)	1142/1374 (83%)	0/854 (0%)	183/235 (78%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	370	THR	HG1	5.72	0.08 – 2.19	21.7
1	A	332	ALA	HB1	0.13	0.14 – 2.58	-5.0
1	A	332	ALA	HB2	0.13	0.14 – 2.58	-5.0
1	A	332	ALA	HB3	0.13	0.14 – 2.58	-5.0

#### 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:

