



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 10:26 AM UTC

PDB ID : 5XBO / pdb_00005xbo
BMRB ID : 36067
Title : Lanthanoid tagging via an unnatural amino acid for protein structure characterization
Authors : Jiang, W.; Gu, X.; Dong, X.; Tang, C.
Deposited on : 2017-03-21

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

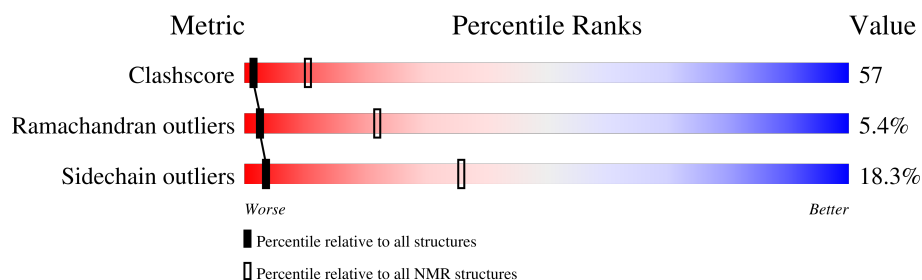
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 12%.

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	76	70% 22% • 5%
2	B	49	8% 43% 24% 6% 18%

2 Ensemble composition and analysis

This entry contains 30 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:72 (72)	0.04	3
2	B:161-B:200 (40)	0.00	14

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 3 single-model clusters were found.

Cluster number	Models
1	2, 8, 9, 10, 13, 16, 20, 24, 25, 29, 30
2	5, 7, 12, 14, 15, 17, 18, 19, 23, 26
3	1, 11, 21, 22, 27, 28
Single-model clusters	3; 4; 6

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1999 atoms, of which 1012 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1232	378	630	105	118	1	

- Molecule 2 is a protein called UV excision repair protein RAD23 homolog A.

Mol	Chain	Residues	Atoms						Trace
2	B	49	Total	C	H	N	O	S	0
			766	240	382	65	76	3	

- Molecule 3 is TERBIUM(III) ION (CCD ID: TB) (formula: Tb).

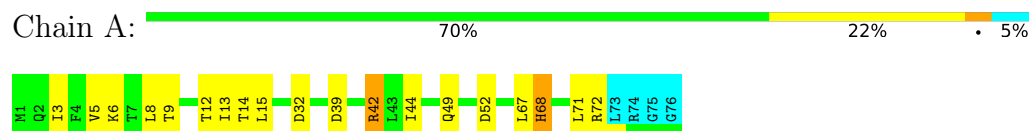
Mol	Chain	Residues	Atoms	
3	A	1	Total	Tb
			1	1

4 Residue-property plots

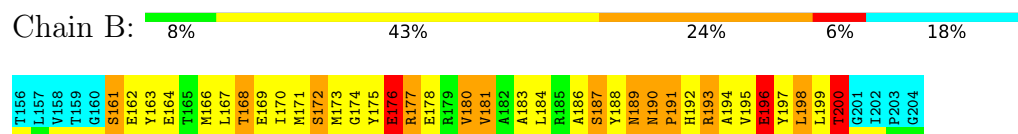
4.1 Average score per residue in the NMR ensemble

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: Polyubiquitin-B



- Molecule 2: UV excision repair protein RAD23 homolog A

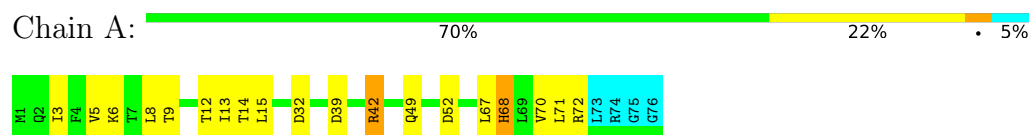


4.2 Scores per residue for each member of the ensemble

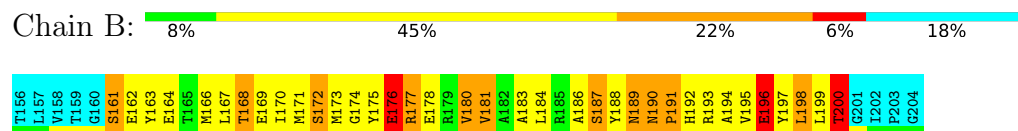
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Polyubiquitin-B



- Molecule 2: UV excision repair protein RAD23 homolog A



4.2.2 Score per residue for model 2

- Molecule 1: Polyubiquitin-B

Chain A: 74% 17% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 12% 37% 27% 6% 18%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Polyubiquitin-B

Chain A: 68% 22% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 43% 22% 8% 18%



4.2.4 Score per residue for model 4

- Molecule 1: Polyubiquitin-B

Chain A: 68% 21% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 10% 41% 22% 8% 18%



4.2.5 Score per residue for model 5

- Molecule 1: Polyubiquitin-B

Chain A: 71% 21% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 39% 29% 6% 18%



4.2.6 Score per residue for model 6

- Molecule 1: Polyubiquitin-B

Chain A: 71% 20% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 41% 27% 6% 18%



4.2.7 Score per residue for model 7

- Molecule 1: Polyubiquitin-B

Chain A: 71% 16% 8% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 41% 27% 6% 18%



4.2.8 Score per residue for model 8

- Molecule 1: Polyubiquitin-B

Chain A: 72% 20% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 10% 39% 27% 6% 18%



4.2.9 Score per residue for model 9

- Molecule 1: Polyubiquitin-B

Chain A: 72% 21% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 43% 24% 6% 18%



4.2.10 Score per residue for model 10

- Molecule 1: Polyubiquitin-B

Chain A: 70% 21% 5%



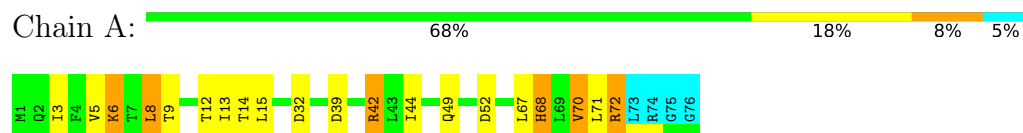
- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 10% 41% 24% 6% 18%

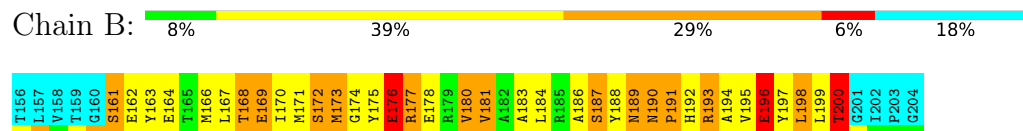


4.2.11 Score per residue for model 11

- Molecule 1: Polyubiquitin-B

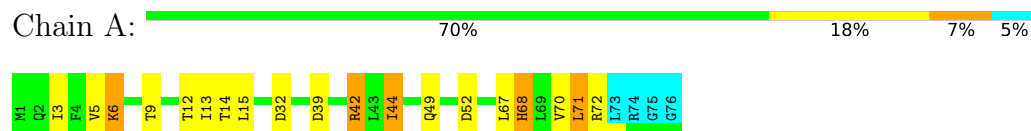


- Molecule 2: UV excision repair protein RAD23 homolog A

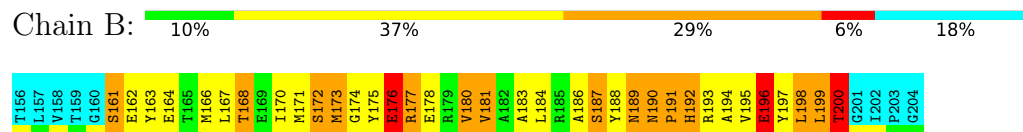


4.2.12 Score per residue for model 12

- Molecule 1: Polyubiquitin-B

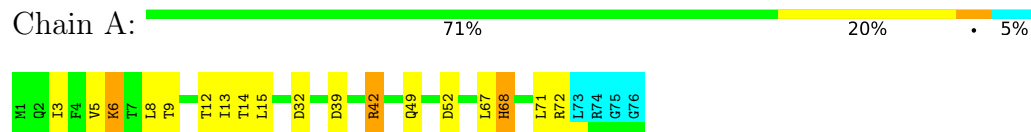


- Molecule 2: UV excision repair protein RAD23 homolog A

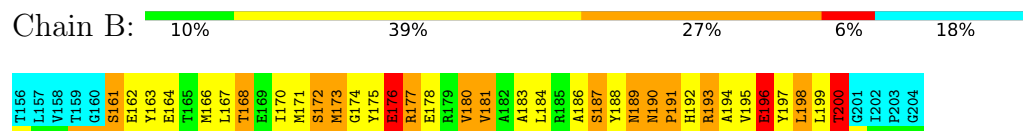


4.2.13 Score per residue for model 13

- Molecule 1: Polyubiquitin-B



- Molecule 2: UV excision repair protein RAD23 homolog A



4.2.14 Score per residue for model 14

- Molecule 1: Polyubiquitin-B

Chain A: 71% 21% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 39% 29% 6% 18%



4.2.15 Score per residue for model 15

- Molecule 1: Polyubiquitin-B

Chain A: 71% 18% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 10% 41% 24% 6% 18%



4.2.16 Score per residue for model 16

- Molecule 1: Polyubiquitin-B

Chain A: 71% 21% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 10% 39% 27% 6% 18%



4.2.17 Score per residue for model 17

- Molecule 1: Polyubiquitin-B

Chain A: 68% 24% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 43% 24% 6% 18%



4.2.18 Score per residue for model 18

- Molecule 1: Polyubiquitin-B

Chain A: 71% 18% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 41% 27% 6% 18%



4.2.19 Score per residue for model 19

- Molecule 1: Polyubiquitin-B

Chain A: 72% 20% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 10% 41% 24% 6% 18%



4.2.20 Score per residue for model 20

- Molecule 1: Polyubiquitin-B

Chain A: 



- Molecule 2: UV excision repair protein RAD23 homolog A

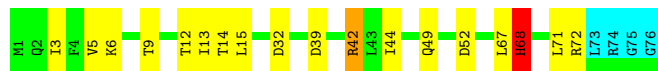
Chain B: 



4.2.21 Score per residue for model 21

- Molecule 1: Polyubiquitin-B

Chain A: 



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 



4.2.22 Score per residue for model 22

- Molecule 1: Polyubiquitin-B

Chain A: 



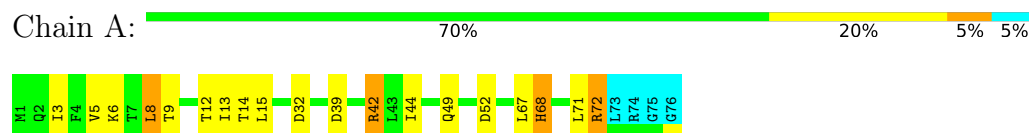
- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 

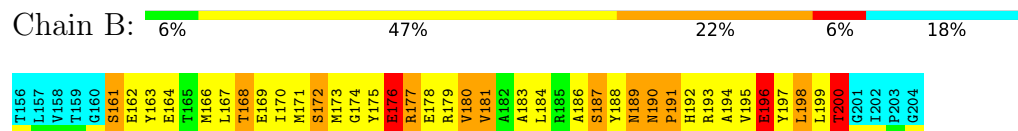


4.2.23 Score per residue for model 23

- Molecule 1: Polyubiquitin-B

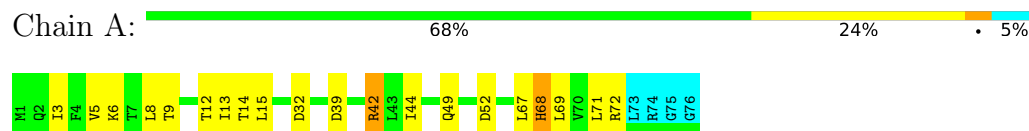


- Molecule 2: UV excision repair protein RAD23 homolog A

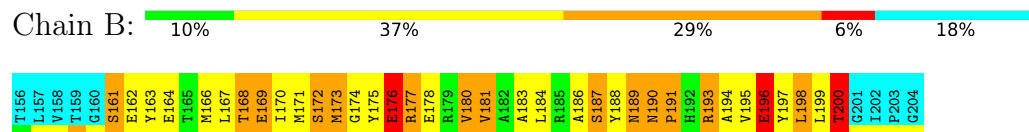


4.2.24 Score per residue for model 24

- Molecule 1: Polyubiquitin-B

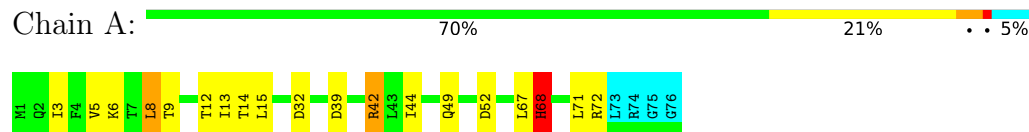


- Molecule 2: UV excision repair protein RAD23 homolog A

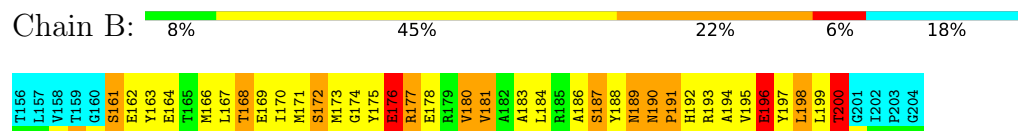


4.2.25 Score per residue for model 25

- Molecule 1: Polyubiquitin-B

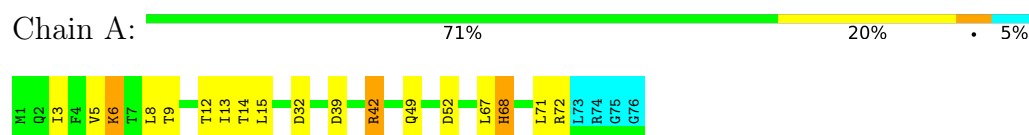


- Molecule 2: UV excision repair protein RAD23 homolog A

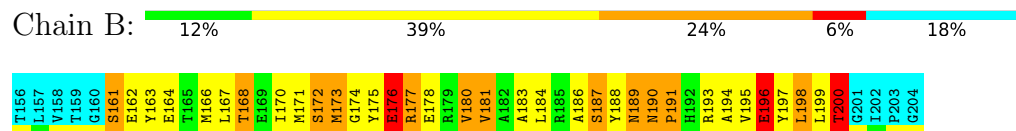


4.2.26 Score per residue for model 26

- Molecule 1: Polyubiquitin-B

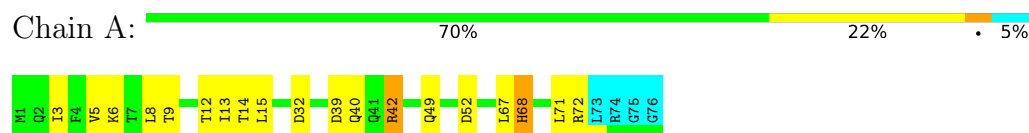


- Molecule 2: UV excision repair protein RAD23 homolog A

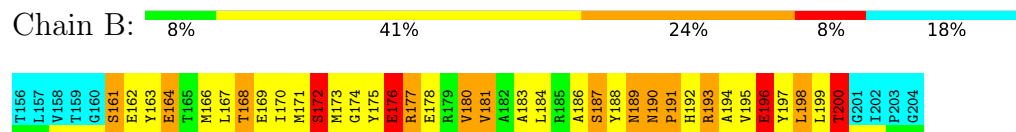


4.2.27 Score per residue for model 27

- Molecule 1: Polyubiquitin-B

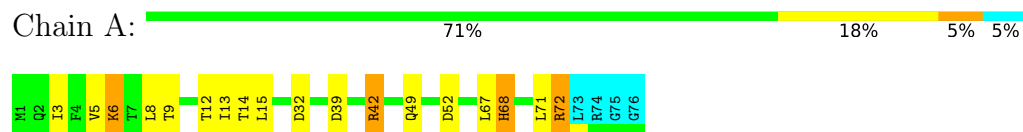


- Molecule 2: UV excision repair protein RAD23 homolog A

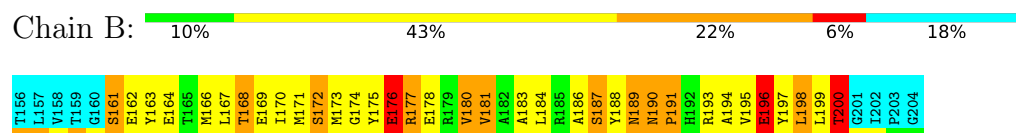


4.2.28 Score per residue for model 28

- Molecule 1: Polyubiquitin-B



- Molecule 2: UV excision repair protein RAD23 homolog A



4.2.29 Score per residue for model 29

- Molecule 1: Polyubiquitin-B

Chain A: 71% 21% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 8% 43% 24% 6% 18%



4.2.30 Score per residue for model 30

- Molecule 1: Polyubiquitin-B

Chain A: 72% 17% 5%



- Molecule 2: UV excision repair protein RAD23 homolog A

Chain B: 10% 39% 27% 6% 18%



5 Refinement protocol and experimental data overview

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

Of the 160 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	6
Total number of shifts	444
Number of shifts mapped to atoms	444
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	1.33±0.00	1±0/581 (0.2± 0.0%)	1.88±0.00	14±0/784 (1.8± 0.0%)
2	B	0.59±0.00	0±0/333 (0.0± 0.0%)	0.92±0.00	1±0/451 (0.2± 0.0%)
All	All	1.12	30/27420 (0.1%)	1.60	448/37050 (1.2%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	42	ARG	C-O	5.30	1.30	1.24	1	30

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	52	ASP	N-CA-C	7.78	120.74	111.33	1	30
1	A	14	THR	CA-CB-OG1	-7.31	98.64	109.60	1	30
1	A	32	ASP	CA-CB-CG	-7.25	105.35	112.60	1	30
1	A	72	ARG	CA-C-O	-7.04	113.38	121.47	25	27
1	A	3	ILE	O-C-N	6.72	130.50	123.04	1	30
1	A	5	VAL	CA-C-O	-6.47	113.36	120.48	1	30
1	A	68	HIS	CA-CB-CG	-6.42	107.38	113.80	11	30
1	A	12	THR	CA-C-N	-6.13	115.19	123.10	1	30
1	A	12	THR	C-N-CA	-6.13	115.19	123.10	1	30
1	A	5	VAL	O-C-N	5.99	129.40	122.99	1	30
1	A	72	ARG	CD-NE-CZ	-5.77	116.32	124.40	23	30
1	A	67	LEU	CA-C-O	-5.58	114.70	121.28	1	30
2	B	196	GLU	N-CA-C	-5.54	105.62	112.38	2	30
1	A	9	THR	CA-CB-OG1	-5.52	101.32	109.60	1	30
1	A	3	ILE	CA-C-O	-5.43	115.97	121.67	1	30
1	A	72	ARG	N-CA-C	-5.31	105.49	111.28	6	1

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	574	600	599	9±3
2	B	327	319	318	100±3
All	All	27060	27570	27510	3095

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ARG:NH2	2:B:199:LEU:HD11	1.00	1.72	1	7
1:A:42:ARG:NH2	2:B:199:LEU:HD21	0.99	1.72	30	9
1:A:42:ARG:NH1	2:B:199:LEU:HD21	0.94	1.77	27	6
1:A:6:LYS:HZ3	1:A:68:HIS:CD2	0.94	1.80	3	1
1:A:42:ARG:NH2	2:B:199:LEU:HD22	0.91	1.80	23	4
2:B:186:ALA:HB1	2:B:197:TYR:CZ	0.90	2.02	9	30
1:A:42:ARG:CZ	2:B:199:LEU:HD21	0.90	1.96	21	12
2:B:171:MET:HE2	2:B:177:ARG:CB	0.90	1.97	30	30
1:A:42:ARG:NH1	2:B:199:LEU:HD13	0.85	1.85	26	4
1:A:42:ARG:NH1	2:B:199:LEU:HD11	0.85	1.87	21	5
1:A:6:LYS:HZ2	1:A:68:HIS:CD2	0.84	1.90	6	1
1:A:42:ARG:CZ	2:B:199:LEU:HD13	0.83	2.03	23	3
1:A:42:ARG:HH12	2:B:199:LEU:HD21	0.83	1.32	10	2
1:A:42:ARG:NH2	2:B:199:LEU:HD12	0.83	1.88	19	5
1:A:44:ILE:HD12	1:A:45:PHE:N	0.82	1.89	22	1
2:B:169:GLU:OE1	2:B:173:MET:HE1	0.82	1.74	28	1
2:B:192:HIS:CG	2:B:193:ARG:HH11	0.81	1.94	13	6
1:A:42:ARG:CZ	2:B:199:LEU:HD11	0.80	2.06	16	7
2:B:192:HIS:CG	2:B:193:ARG:NH1	0.79	2.51	13	6
2:B:163:TYR:CE1	2:B:184:LEU:HD13	0.79	2.13	21	30
1:A:68:HIS:CD2	2:B:173:MET:SD	0.78	2.76	11	4
1:A:6:LYS:NZ	1:A:68:HIS:NE2	0.78	2.32	19	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:192:HIS:ND1	2:B:193:ARG:NH1	0.78	2.32	8	5
1:A:44:ILE:HD12	1:A:44:ILE:C	0.77	2.03	22	1
1:A:6:LYS:NZ	1:A:68:HIS:CD2	0.77	2.52	3	3
1:A:8:LEU:HD23	2:B:192:HIS:CE1	0.77	2.15	29	2
2:B:191:PRO:O	2:B:194:ALA:HB3	0.77	1.80	15	30
1:A:6:LYS:HZ1	1:A:68:HIS:CD2	0.76	1.98	15	1
2:B:192:HIS:CD2	2:B:193:ARG:HH12	0.76	1.97	21	1
2:B:184:LEU:HD23	2:B:190:ASN:O	0.76	1.81	7	30
1:A:6:LYS:HZ2	1:A:68:HIS:CE1	0.73	2.01	30	3
2:B:193:ARG:NH2	2:B:196:GLU:CD	0.73	2.47	6	10
1:A:68:HIS:N	1:A:68:HIS:ND1	0.72	2.35	25	6
2:B:192:HIS:CD2	2:B:193:ARG:NH1	0.72	2.57	21	3
2:B:192:HIS:CE1	2:B:193:ARG:NH1	0.71	2.58	13	2
2:B:196:GLU:O	2:B:200:THR:HG22	0.71	1.86	12	30
1:A:6:LYS:NZ	1:A:68:HIS:CE1	0.70	2.59	30	4
2:B:163:TYR:CD1	2:B:184:LEU:HD13	0.70	2.22	17	30
1:A:42:ARG:HH12	2:B:199:LEU:HD11	0.70	1.45	21	2
1:A:68:HIS:NE2	2:B:173:MET:CE	0.69	2.56	11	1
2:B:171:MET:HE2	2:B:177:ARG:HB2	0.69	1.65	5	30
1:A:8:LEU:O	2:B:192:HIS:NE2	0.69	2.26	15	5
2:B:192:HIS:CG	2:B:193:ARG:HH12	0.69	2.06	21	1
1:A:70:VAL:HG21	2:B:173:MET:HE1	0.69	1.65	1	1
1:A:8:LEU:O	2:B:192:HIS:CE1	0.69	2.46	23	2
2:B:193:ARG:NH1	2:B:196:GLU:OE1	0.68	2.26	26	4
1:A:6:LYS:NZ	2:B:173:MET:SD	0.68	2.67	5	4
1:A:42:ARG:NH2	2:B:172:SER:O	0.68	2.27	3	1
2:B:195:VAL:HA	2:B:198:LEU:HD22	0.68	1.66	25	30
1:A:42:ARG:NH1	2:B:173:MET:SD	0.67	2.67	6	1
1:A:44:ILE:HD11	1:A:70:VAL:CG2	0.67	2.19	17	3
2:B:193:ARG:HH22	2:B:196:GLU:CD	0.66	1.99	3	11
2:B:163:TYR:CE2	2:B:181:VAL:CG2	0.66	2.79	13	30
1:A:8:LEU:HD22	2:B:192:HIS:ND1	0.66	2.06	11	1
2:B:181:VAL:HA	2:B:184:LEU:HD12	0.65	1.69	13	30
2:B:167:LEU:O	2:B:171:MET:HG3	0.65	1.92	19	30
2:B:186:ALA:CB	2:B:197:TYR:CZ	0.65	2.80	21	30
2:B:170:ILE:HG21	2:B:198:LEU:CD2	0.65	2.22	29	30
1:A:68:HIS:ND1	2:B:173:MET:SD	0.65	2.70	27	1
2:B:190:ASN:O	2:B:194:ALA:HB2	0.64	1.93	6	30
1:A:44:ILE:CD1	2:B:173:MET:HE1	0.64	2.21	25	3
1:A:6:LYS:HZ1	2:B:173:MET:HE1	0.64	1.52	24	1
2:B:193:ARG:NH2	2:B:196:GLU:OE1	0.64	2.30	29	16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ARG:HH22	2:B:173:MET:CG	0.64	2.05	6	1
2:B:192:HIS:CE1	2:B:193:ARG:HH12	0.63	2.10	13	3
1:A:8:LEU:HD22	2:B:192:HIS:CG	0.63	2.28	11	1
1:A:44:ILE:C	1:A:44:ILE:CD1	0.63	2.69	22	1
2:B:170:ILE:CG2	2:B:198:LEU:CD2	0.62	2.77	17	30
1:A:6:LYS:NZ	2:B:169:GLU:OE2	0.62	2.27	28	1
1:A:44:ILE:HD12	2:B:173:MET:SD	0.62	2.34	12	2
1:A:8:LEU:HD13	2:B:192:HIS:CE1	0.62	2.29	25	3
1:A:49:GLN:OE1	1:A:72:ARG:NH1	0.62	2.33	30	1
2:B:193:ARG:NH1	2:B:196:GLU:C	0.62	2.58	11	1
1:A:71:LEU:O	1:A:72:ARG:CB	0.61	2.46	4	3
2:B:163:TYR:CE1	2:B:184:LEU:CD1	0.61	2.84	18	30
2:B:188:TYR:O	2:B:189:ASN:CB	0.61	2.49	3	30
2:B:192:HIS:CD2	2:B:193:ARG:HH11	0.61	2.12	22	3
2:B:166:MET:HE1	2:B:189:ASN:OD1	0.61	1.96	5	30
2:B:167:LEU:CD2	2:B:180:VAL:HG22	0.61	2.26	6	30
1:A:42:ARG:HH22	2:B:172:SER:C	0.61	2.03	3	1
2:B:173:MET:HE2	2:B:195:VAL:HG21	0.60	1.74	17	1
1:A:42:ARG:NH2	2:B:199:LEU:CD1	0.60	2.65	5	4
2:B:170:ILE:HA	2:B:173:MET:HE3	0.59	1.74	6	1
1:A:42:ARG:HH22	2:B:199:LEU:HD21	0.59	1.55	29	4
1:A:8:LEU:H	1:A:8:LEU:CD1	0.59	2.09	29	1
2:B:176:GLU:O	2:B:180:VAL:HG12	0.58	1.99	5	30
2:B:193:ARG:HH11	2:B:196:GLU:CD	0.58	2.07	2	2
1:A:42:ARG:CZ	2:B:199:LEU:CD1	0.57	2.82	2	4
1:A:42:ARG:NH2	2:B:173:MET:SD	0.57	2.77	6	1
1:A:8:LEU:HD22	2:B:192:HIS:CE1	0.57	2.34	10	2
1:A:8:LEU:HD13	2:B:192:HIS:CD2	0.57	2.35	13	2
1:A:68:HIS:N	1:A:68:HIS:CD2	0.57	2.73	18	1
2:B:195:VAL:HA	2:B:198:LEU:CD2	0.56	2.31	19	30
1:A:42:ARG:NH1	2:B:199:LEU:HD12	0.56	2.15	2	1
2:B:169:GLU:O	2:B:173:MET:HE2	0.56	2.01	23	1
2:B:183:ALA:O	2:B:187:SER:N	0.55	2.40	18	30
2:B:193:ARG:NE	2:B:193:ARG:CA	0.55	2.70	16	7
2:B:167:LEU:O	2:B:171:MET:CB	0.55	2.55	12	30
1:A:42:ARG:HE	1:A:49:GLN:NE2	0.55	2.00	1	30
2:B:169:GLU:OE2	2:B:173:MET:CE	0.55	2.54	6	1
2:B:171:MET:CE	2:B:177:ARG:HB2	0.55	2.32	1	30
1:A:44:ILE:O	1:A:68:HIS:ND1	0.55	2.40	10	1
2:B:193:ARG:HH11	2:B:197:TYR:CA	0.55	2.15	11	1
2:B:193:ARG:HH11	2:B:197:TYR:N	0.55	2.00	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ARG:CZ	2:B:199:LEU:HD22	0.55	2.32	26	2
2:B:163:TYR:CE2	2:B:181:VAL:HG22	0.54	2.38	1	30
2:B:184:LEU:CD2	2:B:190:ASN:O	0.54	2.55	22	30
2:B:170:ILE:CG2	2:B:198:LEU:HD23	0.54	2.33	11	30
2:B:171:MET:CE	2:B:177:ARG:CB	0.54	2.83	22	30
2:B:170:ILE:HG23	2:B:195:VAL:HB	0.54	1.80	6	30
1:A:8:LEU:CD1	1:A:8:LEU:N	0.54	2.70	29	1
2:B:167:LEU:O	2:B:171:MET:N	0.54	2.41	6	30
2:B:171:MET:C	2:B:173:MET:N	0.54	2.66	6	30
2:B:163:TYR:CZ	2:B:181:VAL:HG22	0.54	2.38	23	30
2:B:180:VAL:O	2:B:184:LEU:HG	0.54	2.03	29	30
2:B:199:LEU:CD2	2:B:199:LEU:C	0.54	2.81	12	4
1:A:68:HIS:NE2	2:B:173:MET:HE3	0.54	2.16	11	1
2:B:196:GLU:HA	2:B:199:LEU:HD12	0.54	1.79	6	1
2:B:193:ARG:NH1	2:B:197:TYR:N	0.54	2.55	11	1
1:A:8:LEU:CD1	2:B:192:HIS:CE1	0.53	2.91	1	2
2:B:169:GLU:OE2	2:B:173:MET:HE1	0.53	2.02	6	1
2:B:162:GLU:O	2:B:166:MET:CG	0.53	2.57	2	30
2:B:170:ILE:CG2	2:B:195:VAL:HB	0.53	2.34	22	30
2:B:187:SER:O	2:B:188:TYR:CB	0.53	2.57	13	30
2:B:190:ASN:ND2	2:B:190:ASN:N	0.53	2.57	23	30
2:B:199:LEU:C	2:B:199:LEU:HD23	0.53	2.29	19	5
1:A:68:HIS:ND1	1:A:69:LEU:N	0.53	2.56	24	1
2:B:191:PRO:O	2:B:194:ALA:CB	0.53	2.57	15	30
1:A:44:ILE:HD11	1:A:70:VAL:HG21	0.53	1.79	17	1
1:A:6:LYS:HZ1	1:A:68:HIS:HB3	0.53	1.64	7	1
2:B:183:ALA:O	2:B:187:SER:HB3	0.52	2.05	7	30
1:A:8:LEU:HD22	2:B:192:HIS:NE2	0.52	2.19	20	2
2:B:171:MET:O	2:B:173:MET:N	0.52	2.43	4	30
1:A:44:ILE:HD12	2:B:173:MET:HE1	0.52	1.81	25	1
1:A:44:ILE:HG13	2:B:173:MET:HE1	0.52	1.80	21	1
2:B:192:HIS:CD2	2:B:192:HIS:C	0.52	2.88	12	1
2:B:171:MET:O	2:B:172:SER:C	0.51	2.54	1	30
1:A:6:LYS:CE	2:B:173:MET:SD	0.51	2.99	23	1
2:B:166:MET:CE	2:B:189:ASN:OD1	0.51	2.59	13	30
2:B:167:LEU:O	2:B:171:MET:CG	0.51	2.59	3	30
1:A:42:ARG:HG2	1:A:44:ILE:HD11	0.51	1.83	7	2
2:B:199:LEU:C	2:B:199:LEU:CD2	0.51	2.84	19	1
2:B:187:SER:O	2:B:190:ASN:OD1	0.50	2.30	1	30
2:B:173:MET:O	2:B:175:TYR:CD1	0.50	2.65	6	12
2:B:171:MET:HE2	2:B:177:ARG:HB3	0.50	1.82	29	30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:169:GLU:OE2	2:B:173:MET:SD	0.50	2.70	3	1
1:A:8:LEU:CD1	2:B:192:HIS:NE2	0.50	2.74	13	2
1:A:6:LYS:CD	1:A:6:LYS:C	0.50	2.84	30	1
1:A:42:ARG:CZ	2:B:199:LEU:HD12	0.49	2.35	2	2
1:A:42:ARG:HH22	2:B:199:LEU:HD11	0.49	1.65	17	1
2:B:166:MET:HE1	2:B:189:ASN:O	0.49	2.08	19	30
1:A:42:ARG:NH1	2:B:173:MET:CE	0.49	2.75	3	1
2:B:199:LEU:O	2:B:200:THR:C	0.49	2.56	1	30
1:A:8:LEU:HD23	2:B:192:HIS:NE2	0.49	2.22	17	2
2:B:169:GLU:CD	2:B:169:GLU:C	0.49	2.80	18	2
2:B:176:GLU:O	2:B:180:VAL:CG1	0.48	2.61	25	30
2:B:186:ALA:HB1	2:B:197:TYR:CE1	0.48	2.44	15	30
2:B:175:TYR:CE2	2:B:195:VAL:HG23	0.48	2.44	27	18
2:B:173:MET:O	2:B:175:TYR:CD2	0.48	2.66	11	18
2:B:181:VAL:HA	2:B:184:LEU:CD1	0.48	2.39	3	30
2:B:195:VAL:O	2:B:199:LEU:HD13	0.48	2.08	29	5
1:A:42:ARG:NE	2:B:199:LEU:HD21	0.48	2.20	21	1
2:B:175:TYR:CD1	2:B:198:LEU:HG	0.48	2.44	13	18
1:A:42:ARG:HH12	2:B:173:MET:HE3	0.48	1.67	3	1
2:B:174:GLY:O	2:B:175:TYR:CD2	0.48	2.67	19	12
1:A:68:HIS:CE1	2:B:173:MET:HE3	0.48	2.43	11	2
1:A:8:LEU:CD2	2:B:192:HIS:CE1	0.47	2.97	17	3
2:B:167:LEU:HD13	2:B:177:ARG:O	0.47	2.10	3	30
2:B:177:ARG:CZ	2:B:177:ARG:HB3	0.47	2.40	5	22
2:B:193:ARG:NH2	2:B:196:GLU:CG	0.47	2.78	15	6
2:B:177:ARG:HB3	2:B:177:ARG:CZ	0.47	2.39	27	8
2:B:176:GLU:OE1	2:B:178:GLU:CD	0.47	2.58	1	30
2:B:192:HIS:CB	2:B:193:ARG:NH2	0.47	2.78	19	1
2:B:177:ARG:O	2:B:181:VAL:HB	0.46	2.11	4	30
1:A:6:LYS:HZ1	2:B:173:MET:CE	0.46	2.20	24	1
2:B:166:MET:SD	2:B:189:ASN:O	0.46	2.74	12	30
2:B:195:VAL:HA	2:B:198:LEU:HB2	0.46	1.88	11	30
2:B:187:SER:O	2:B:188:TYR:HB2	0.46	2.11	21	30
2:B:168:THR:C	2:B:171:MET:HB2	0.46	2.36	25	30
2:B:171:MET:HE2	2:B:177:ARG:CA	0.46	2.41	1	30
2:B:186:ALA:HB1	2:B:197:TYR:OH	0.46	2.11	3	30
1:A:44:ILE:HD11	1:A:70:VAL:HG23	0.46	1.86	4	2
1:A:6:LYS:CD	1:A:68:HIS:CD2	0.46	2.98	11	1
1:A:6:LYS:CE	1:A:68:HIS:NE2	0.46	2.78	19	2
1:A:71:LEU:O	2:B:196:GLU:OE2	0.46	2.34	12	1
1:A:8:LEU:CD1	2:B:192:HIS:CD2	0.46	2.99	22	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:188:TYR:O	2:B:189:ASN:HB2	0.46	2.11	6	30
2:B:175:TYR:CD2	2:B:198:LEU:HG	0.46	2.46	3	12
2:B:193:ARG:NE	2:B:193:ARG:HA	0.45	2.27	19	6
1:A:42:ARG:HH21	2:B:199:LEU:HD22	0.45	1.64	23	1
1:A:42:ARG:HH12	2:B:199:LEU:CD2	0.45	2.14	10	1
2:B:167:LEU:HD22	2:B:180:VAL:HG22	0.45	1.89	17	30
2:B:162:GLU:O	2:B:166:MET:HG3	0.45	2.12	3	30
2:B:196:GLU:O	2:B:200:THR:CG2	0.45	2.64	8	29
2:B:175:TYR:CE1	2:B:195:VAL:HG23	0.45	2.47	19	12
2:B:173:MET:HE3	2:B:195:VAL:HG21	0.45	1.88	16	1
2:B:174:GLY:O	2:B:175:TYR:CD1	0.45	2.70	26	18
1:A:42:ARG:NH1	2:B:199:LEU:CD1	0.45	2.71	26	2
1:A:8:LEU:H	1:A:8:LEU:HD12	0.44	1.69	29	1
2:B:192:HIS:CG	2:B:193:ARG:CZ	0.44	3.01	21	1
1:A:6:LYS:HZ3	1:A:68:HIS:CE1	0.44	2.30	24	1
2:B:195:VAL:C	2:B:197:TYR:N	0.44	2.75	17	25
2:B:171:MET:O	2:B:174:GLY:N	0.44	2.51	17	30
2:B:197:TYR:HA	2:B:200:THR:HG23	0.44	1.90	12	30
1:A:68:HIS:CE1	1:A:70:VAL:HG23	0.44	2.48	11	1
1:A:68:HIS:NE2	2:B:173:MET:SD	0.44	2.91	11	1
2:B:184:LEU:HD23	2:B:194:ALA:HB2	0.43	1.90	12	30
2:B:187:SER:O	2:B:188:TYR:CD1	0.43	2.72	26	30
1:A:8:LEU:HD13	2:B:192:HIS:NE2	0.43	2.28	22	2
2:B:170:ILE:HA	2:B:173:MET:HE2	0.43	1.89	28	1
2:B:173:MET:CE	2:B:195:VAL:HG21	0.43	2.41	17	1
1:A:6:LYS:NZ	2:B:169:GLU:OE1	0.43	2.50	9	1
2:B:193:ARG:HH11	2:B:196:GLU:HB3	0.43	1.73	17	1
2:B:167:LEU:O	2:B:171:MET:HB2	0.43	2.14	4	30
1:A:70:VAL:HG11	2:B:172:SER:HA	0.43	1.91	3	1
1:A:6:LYS:NZ	1:A:68:HIS:CG	0.43	2.87	3	1
2:B:173:MET:O	2:B:175:TYR:CE1	0.43	2.71	6	11
2:B:192:HIS:HB3	2:B:193:ARG:HH22	0.43	1.73	27	1
2:B:170:ILE:O	2:B:175:TYR:HB2	0.43	2.14	11	30
2:B:192:HIS:HB2	2:B:193:ARG:NH2	0.43	2.28	19	1
2:B:166:MET:CE	2:B:189:ASN:O	0.42	2.68	5	30
2:B:168:THR:HA	2:B:171:MET:HB2	0.42	1.91	17	30
2:B:197:TYR:C	2:B:199:LEU:N	0.42	2.77	4	24
1:A:42:ARG:HH22	2:B:173:MET:HG3	0.42	1.71	6	1
2:B:195:VAL:O	2:B:198:LEU:HB2	0.42	2.15	22	30
1:A:68:HIS:CE1	2:B:173:MET:SD	0.42	3.12	27	1
2:B:168:THR:O	2:B:171:MET:HB2	0.42	2.15	8	30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:175:TYR:O	2:B:176:GLU:C	0.42	2.63	29	28
1:A:6:LYS:HD2	1:A:68:HIS:CD2	0.42	2.49	11	3
2:B:168:THR:CA	2:B:171:MET:HB2	0.42	2.45	20	30
2:B:191:PRO:O	2:B:194:ALA:N	0.42	2.53	3	30
2:B:193:ARG:O	2:B:197:TYR:HB2	0.42	2.15	22	30
2:B:193:ARG:NH2	2:B:196:GLU:HB2	0.42	2.30	4	4
2:B:181:VAL:HG23	2:B:184:LEU:HD12	0.42	1.92	4	24
1:A:42:ARG:NH1	2:B:173:MET:HE3	0.42	2.30	3	1
2:B:166:MET:HB3	2:B:191:PRO:HB3	0.42	1.92	12	23
2:B:169:GLU:C	2:B:171:MET:N	0.42	2.78	1	17
1:A:42:ARG:CZ	2:B:173:MET:SD	0.42	3.08	6	1
2:B:192:HIS:CG	2:B:193:ARG:NH2	0.42	2.87	21	1
1:A:68:HIS:CD2	2:B:173:MET:HG3	0.42	2.50	1	1
2:B:181:VAL:O	2:B:184:LEU:HB2	0.41	2.15	8	26
1:A:8:LEU:HD13	2:B:192:HIS:ND1	0.41	2.31	10	1
1:A:6:LYS:NZ	2:B:173:MET:CE	0.41	2.83	24	1
1:A:6:LYS:HD2	1:A:68:HIS:ND1	0.41	2.29	12	1
2:B:162:GLU:O	2:B:166:MET:HG2	0.41	2.16	22	23
2:B:187:SER:C	2:B:188:TYR:CG	0.41	2.99	1	11
2:B:192:HIS:HB3	2:B:193:ARG:HH11	0.41	1.74	9	1
1:A:42:ARG:HH12	2:B:173:MET:CG	0.41	2.29	6	1
1:A:42:ARG:CZ	2:B:199:LEU:CD2	0.41	2.99	26	2
2:B:161:SER:O	2:B:162:GLU:C	0.41	2.64	7	12
2:B:167:LEU:N	2:B:167:LEU:HD23	0.41	2.31	25	8
2:B:167:LEU:HD23	2:B:167:LEU:N	0.41	2.31	30	2
2:B:169:GLU:O	2:B:172:SER:OG	0.41	2.36	24	1
2:B:163:TYR:CZ	2:B:181:VAL:CG2	0.40	3.05	18	3
2:B:173:MET:O	2:B:175:TYR:CE2	0.40	2.75	18	1
2:B:193:ARG:HA	2:B:193:ARG:NE	0.40	2.31	2	1
2:B:193:ARG:HG3	2:B:193:ARG:NH2	0.40	2.30	17	1
1:A:6:LYS:HE2	1:A:68:HIS:ND1	0.40	2.31	23	1
1:A:70:VAL:HG21	2:B:173:MET:CE	0.40	2.43	1	1
2:B:167:LEU:HD23	2:B:180:VAL:HG22	0.40	1.94	6	2
2:B:193:ARG:CA	2:B:193:ARG:NE	0.40	2.84	25	1
1:A:6:LYS:HG2	1:A:68:HIS:NE2	0.40	2.31	30	1
1:A:44:ILE:HD12	1:A:45:PHE:CA	0.40	2.46	22	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	71/76 (93%)	71±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	40/49 (82%)	27±0 (68±0%)	7±0 (18±0%)	6±0 (15±0%)	0	4
All	All	3330/3750 (89%)	2937 (88%)	212 (6%)	181 (5%)	2	22

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	161	SER	30
2	B	172	SER	30
2	B	176	GLU	30
2	B	189	ASN	30
2	B	191	PRO	30
2	B	200	THR	30
1	A	72	ARG	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	66/68 (97%)	60±1 (91±1%)	6±1 (9±1%)	11	58
2	B	35/41 (85%)	22±1 (64±3%)	13±1 (36±3%)	1	8
All	All	3030/3270 (93%)	2475 (82%)	555 (18%)	3	36

All 26 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	13	ILE	30
1	A	15	LEU	30
1	A	39	ASP	30
1	A	71	LEU	30
2	B	164	GLU	30
2	B	168	THR	30
2	B	176	GLU	30
2	B	177	ARG	30
2	B	180	VAL	30
2	B	181	VAL	30
2	B	187	SER	30
2	B	190	ASN	30
2	B	196	GLU	30
2	B	198	LEU	30
2	B	200	THR	30
2	B	193	ARG	19
1	A	8	LEU	18
1	A	6	LYS	17
2	B	173	MET	14
1	A	44	ILE	9
1	A	68	HIS	9
2	B	192	HIS	6
2	B	169	GLU	5
2	B	199	LEU	4
2	B	172	SER	3
1	A	70	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 12% for the well-defined parts and 11% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *uba-ctrl.star*

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	62
Number of shifts mapped to atoms	62
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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}N	31	0.96 ± 0.94	None needed (imprecise)

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 4%, i.e. 62 atoms were assigned a chemical shift out of a possible 1582. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	62/557 (11%)	31/225 (14%)	0/224 (0%)	31/108 (29%)
Sidechain	0/944 (0%)	0/612 (0%)	0/294 (0%)	0/38 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	62/1582 (4%)	31/875 (4%)	0/557 (0%)	31/150 (21%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 62 atoms were assigned a chemical shift out of a possible 1738. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	62/625 (10%)	31/255 (12%)	0/250 (0%)	31/120 (26%)
Sidechain	0/1032 (0%)	0/671 (0%)	0/320 (0%)	0/41 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	62/1738 (4%)	31/964 (3%)	0/609 (0%)	31/165 (19%)

7.1.4 Statistically unusual chemical shifts [i](#)

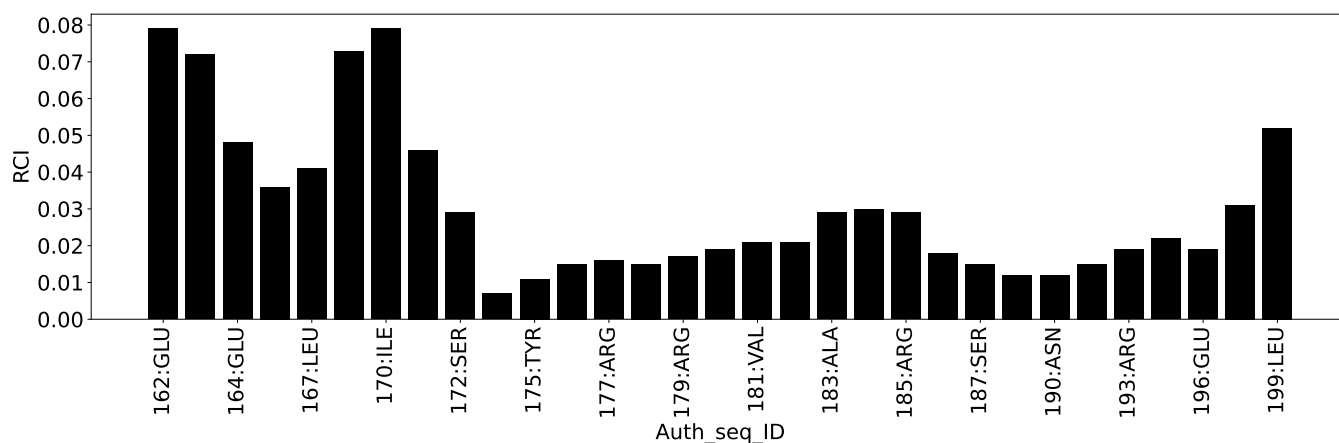
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	174	GLY	N	131.06	91.59 – 127.52	6.0

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 B:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *ubac1_tm.star*

7.2.1 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	58
Number of shifts mapped to atoms	58
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.2.2 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	29	1.10 ± 0.99	None needed (imprecise)

7.2.3 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 4%, i.e. 58 atoms were assigned a chemical shift out of a possible 1582. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	58/557 (10%)	29/225 (13%)	0/224 (0%)	29/108 (27%)
Sidechain	0/944 (0%)	0/612 (0%)	0/294 (0%)	0/38 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	58/1582 (4%)	29/875 (3%)	0/557 (0%)	29/150 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 58 atoms were assigned a chemical shift out of a possible 1738. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	58/625 (9%)	29/255 (11%)	0/250 (0%)	29/120 (24%)
Sidechain	0/1032 (0%)	0/671 (0%)	0/320 (0%)	0/41 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	58/1738 (3%)	29/964 (3%)	0/609 (0%)	29/165 (18%)

7.2.4 Statistically unusual chemical shifts [i](#)

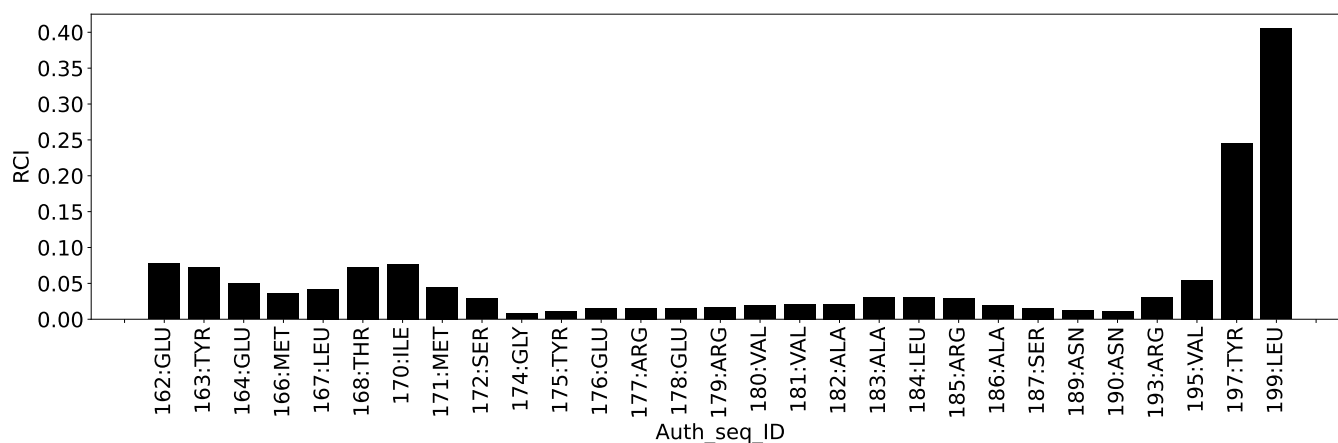
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	174	GLY	N	131.17	91.59 – 127.52	6.0

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 B:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *ubac1_tb.star*

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	62
Number of shifts mapped to atoms	62
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.3.2 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	31	0.88 ± 0.67	None needed (imprecise)

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 4%, i.e. 62 atoms were assigned a chemical shift out of a possible 1582. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	62/557 (11%)	31/225 (14%)	0/224 (0%)	31/108 (29%)
Sidechain	0/944 (0%)	0/612 (0%)	0/294 (0%)	0/38 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	62/1582 (4%)	31/875 (4%)	0/557 (0%)	31/150 (21%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 62 atoms were assigned a chemical shift out of a possible 1738. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	62/625 (10%)	31/255 (12%)	0/250 (0%)	31/120 (26%)
Sidechain	0/1032 (0%)	0/671 (0%)	0/320 (0%)	0/41 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	62/1738 (4%)	31/964 (3%)	0/609 (0%)	31/165 (19%)

7.3.4 Statistically unusual chemical shifts [i](#)

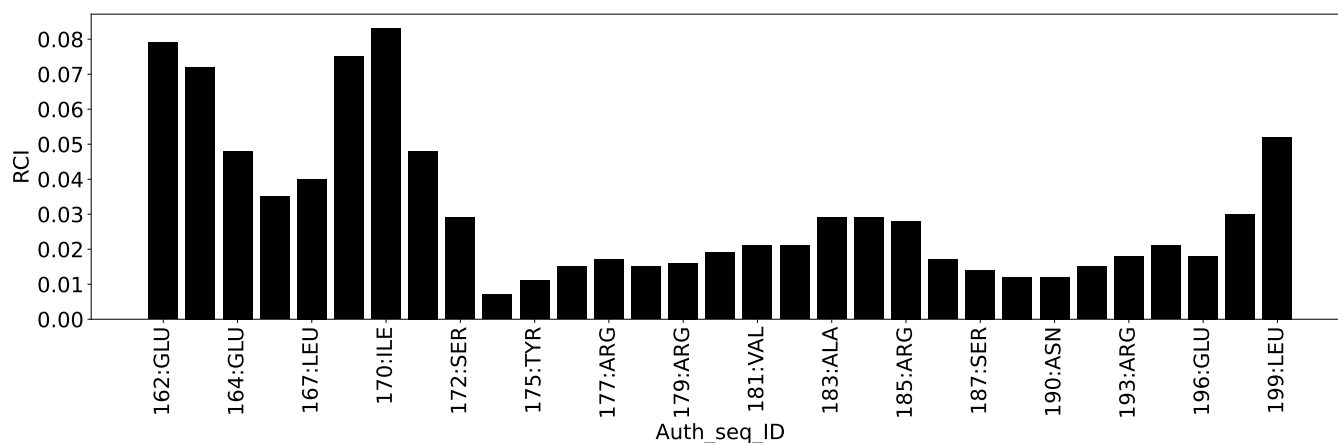
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
3	B	174	GLY	N	130.97	91.59 – 127.52	6.0

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 B:



7.4 Chemical shift list 4

File name: working_cs.cif

Chemical shift list name: *ubc1tm.star*

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	64
Number of shifts mapped to atoms	64
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	32	-0.70 ± 0.75	None needed (imprecise)

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 4%, i.e. 58 atoms were assigned a chemical shift out of a possible 1582. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	58/557 (10%)	29/225 (13%)	0/224 (0%)	29/108 (27%)
Sidechain	0/944 (0%)	0/612 (0%)	0/294 (0%)	0/38 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	58/1582 (4%)	29/875 (3%)	0/557 (0%)	29/150 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 64 atoms were assigned a chemical shift out of a possible 1738. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	64/625 (10%)	32/255 (13%)	0/250 (0%)	32/120 (27%)
Sidechain	0/1032 (0%)	0/671 (0%)	0/320 (0%)	0/41 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	64/1738 (4%)	32/964 (3%)	0/609 (0%)	32/165 (19%)

7.4.4 Statistically unusual chemical shifts [i](#)

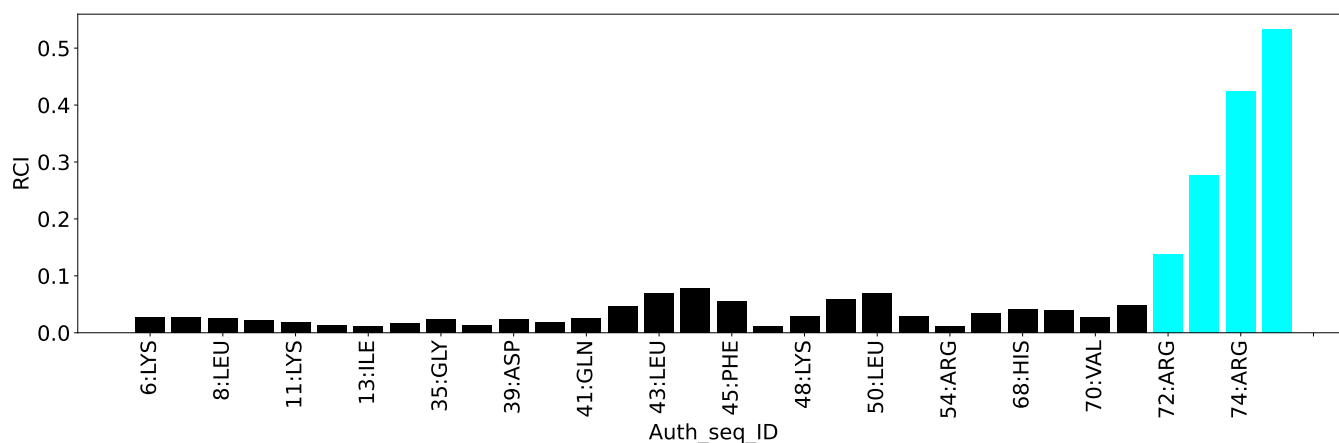
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
4	A	47	GLY	N	128.32	91.59 – 127.52	5.2

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:



7.5 Chemical shift list 5

File name: working_cs.cif

Chemical shift list name: *ubc1tb.star*

7.5.1 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	64
Number of shifts mapped to atoms	64
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.5.2 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	32	-0.70 ± 0.75	None needed (imprecise)

7.5.3 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 4%, i.e. 58 atoms were assigned a chemical shift out of a possible 1582. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	58/557 (10%)	29/225 (13%)	0/224 (0%)	29/108 (27%)
Sidechain	0/944 (0%)	0/612 (0%)	0/294 (0%)	0/38 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	58/1582 (4%)	29/875 (3%)	0/557 (0%)	29/150 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 64 atoms were assigned a chemical shift out of a possible 1738. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	64/625 (10%)	32/255 (13%)	0/250 (0%)	32/120 (27%)
Sidechain	0/1032 (0%)	0/671 (0%)	0/320 (0%)	0/41 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	64/1738 (4%)	32/964 (3%)	0/609 (0%)	32/165 (19%)

7.5.4 Statistically unusual chemical shifts [i](#)

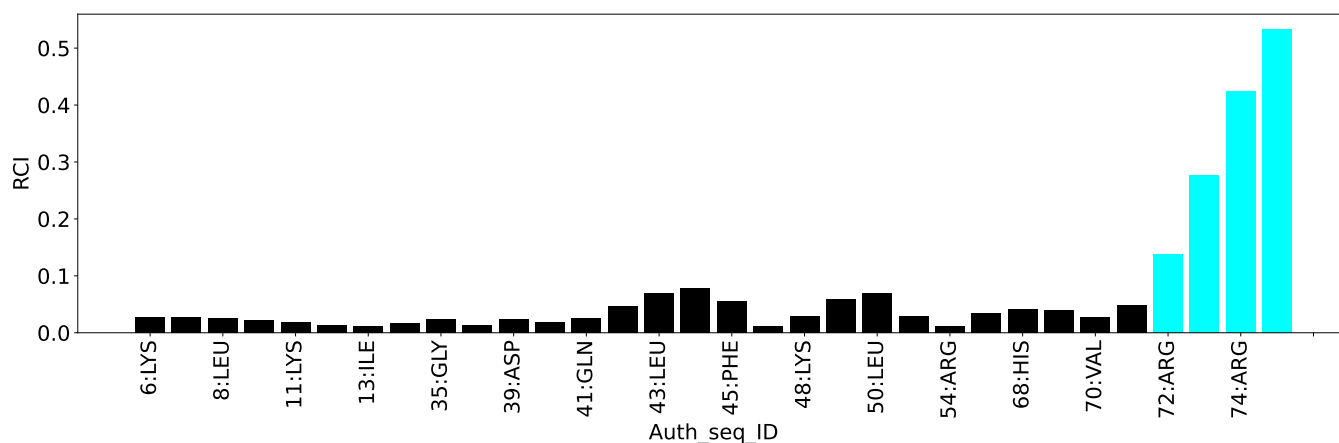
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
5	A	47	GLY	N	128.32	91.59 – 127.52	5.2

7.5.5 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:



7.6 Chemical shift list 6

File name: working_cs.cif

Chemical shift list name: *ubctrl.star*

7.6.1 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	134
Number of shifts mapped to atoms	134
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.6.2 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	67	0.65 ± 0.53	None needed (imprecise)

7.6.3 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 8%, i.e. 128 atoms were assigned a chemical shift out of a possible 1582. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	128/557 (23%)	64/225 (28%)	0/224 (0%)	64/108 (59%)
Sidechain	0/944 (0%)	0/612 (0%)	0/294 (0%)	0/38 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	128/1582 (8%)	64/875 (7%)	0/557 (0%)	64/150 (43%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 134 atoms were assigned a chemical shift out of a possible 1738. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	134/625 (21%)	67/255 (26%)	0/250 (0%)	67/120 (56%)
Sidechain	0/1032 (0%)	0/671 (0%)	0/320 (0%)	0/41 (0%)
Aromatic	0/81 (0%)	0/38 (0%)	0/39 (0%)	0/4 (0%)
Overall	134/1738 (8%)	67/964 (7%)	0/609 (0%)	67/165 (41%)

7.6.4 Statistically unusual chemical shifts [i](#)

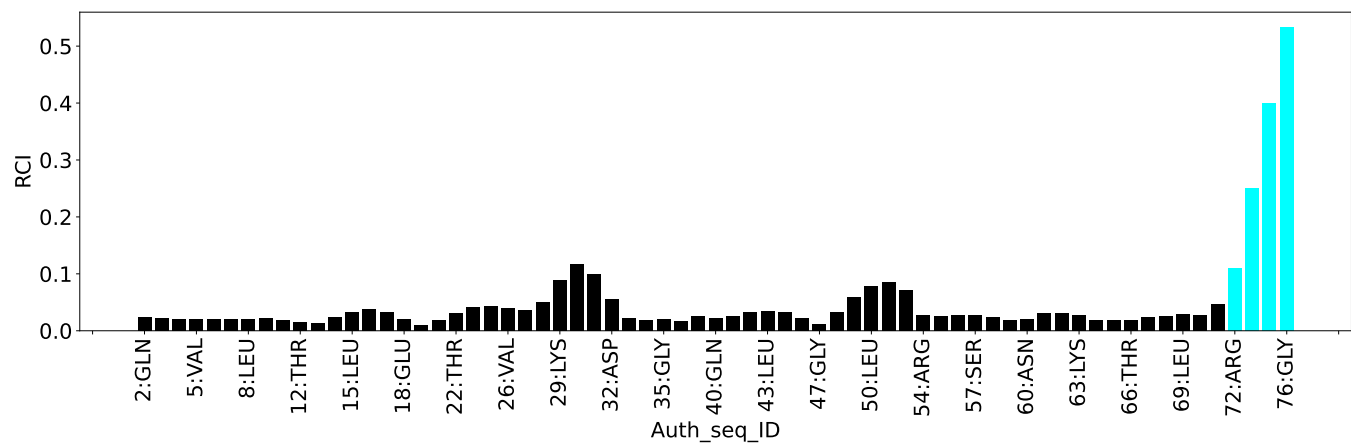
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
6	A	47	GLY	N	128.65	91.59 – 127.52	5.3

7.6.5 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:



8 NMR restraints analysis

No restraints data found

9 Distance violation analysis ⓘ

No distance restraints data found

10 Dihedral-angle violation analysis

No dihedral-angle restraints found