



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:59 pm GMT

PDB ID : 1T4N
Title : Solution structure of Rnt1p dsRBD
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Deposited on : 2004-04-30

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

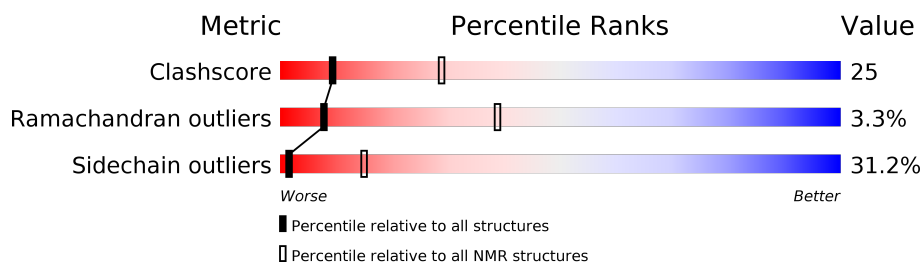
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	94	

2 Ensemble composition and analysis

This entry contains 51 models. Model 47 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:369-A:389, A:399-A:406, A:410-A:446 (66)	0.22	47

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 6 clusters and 6 single-model clusters were found.

Cluster number	Models
1	1, 10, 11, 12, 14, 16, 19, 22, 26, 28, 30, 31, 32, 33, 37, 39, 40, 41, 42, 43, 45, 47, 49
2	2, 8, 15, 17, 21, 24, 34
3	3, 6, 23, 29, 46
4	4, 13, 20, 36, 44
5	5, 9, 50
6	18, 48
Single-model clusters	7; 25; 27; 35; 38; 51

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1369 atoms, of which 697 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribonuclease III.

Mol	Chain	Residues	Atoms						Trace
1	A	88	Total	C	H	N	O	S	0
			1369	422	697	125	121	4	

There are 10 discrepancies between the modelled and reference sequences:

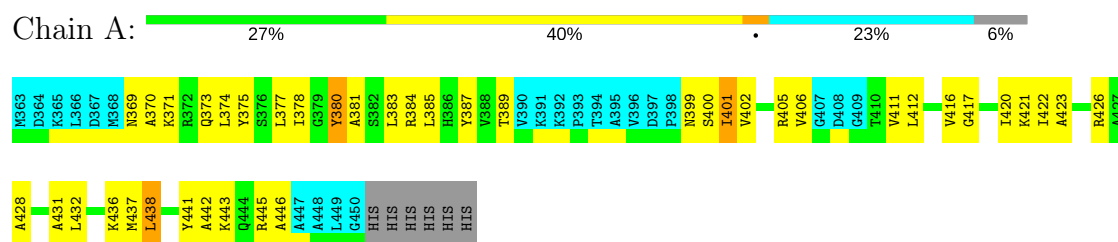
Chain	Residue	Modelled	Actual	Comment	Reference
A	363	MET	-	INITIATING METHIONINE	UNP Q02555
A	448	ALA	-	EXPRESSION TAG	UNP Q02555
A	449	LEU	-	EXPRESSION TAG	UNP Q02555
A	450	GLY	-	EXPRESSION TAG	UNP Q02555
A	451	HIS	-	EXPRESSION TAG	UNP Q02555
A	452	HIS	-	EXPRESSION TAG	UNP Q02555
A	453	HIS	-	EXPRESSION TAG	UNP Q02555
A	454	HIS	-	EXPRESSION TAG	UNP Q02555
A	455	HIS	-	EXPRESSION TAG	UNP Q02555
A	456	HIS	-	EXPRESSION TAG	UNP Q02555

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Ribonuclease III

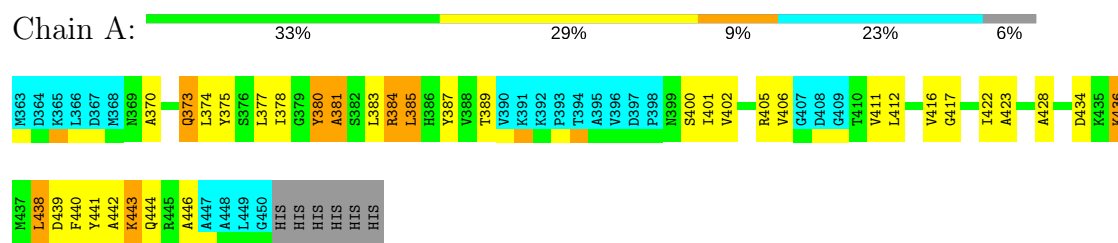


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

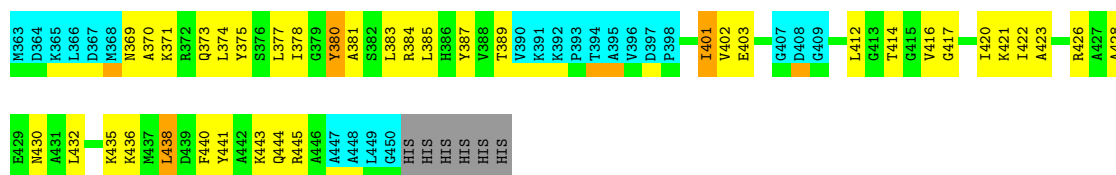
- Molecule 1: Ribonuclease III



4.2.2 Score per residue for model 2

- Molecule 1: Ribonuclease III

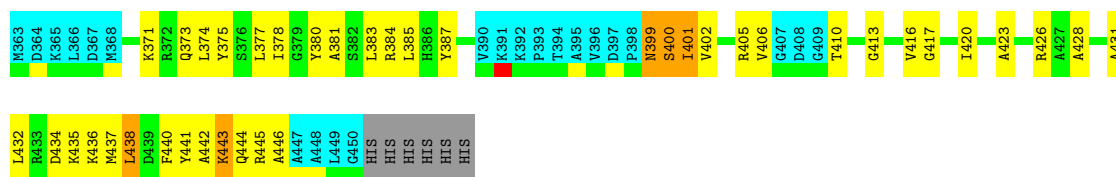




4.2.3 Score per residue for model 3

- Molecule 1: Ribonuclease III

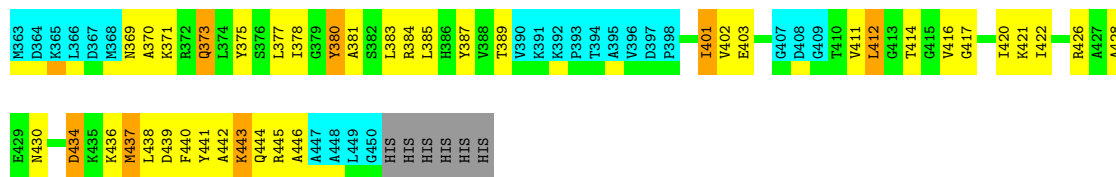
Chain A: 28% 37% 5% 23% 6%



4.2.4 Score per residue for model 4

- Molecule 1: Ribonuclease III

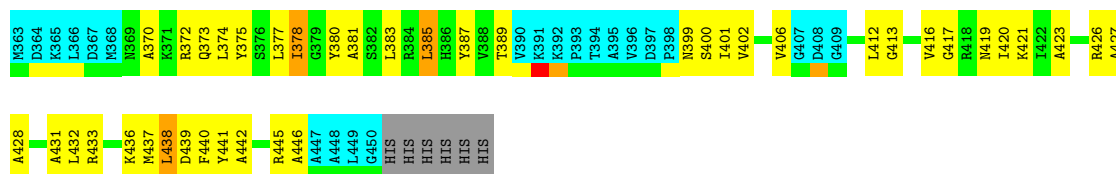
Chain A: 28% 35% 7% 23% 6%



4.2.5 Score per residue for model 5

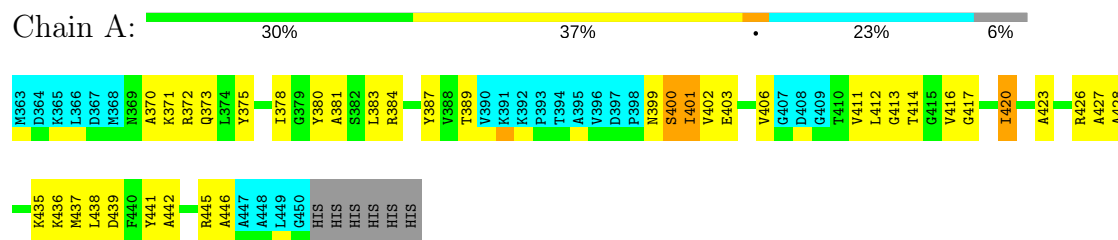
- Molecule 1: Ribonuclease III

Chain A: 27% 40% 23% 6%



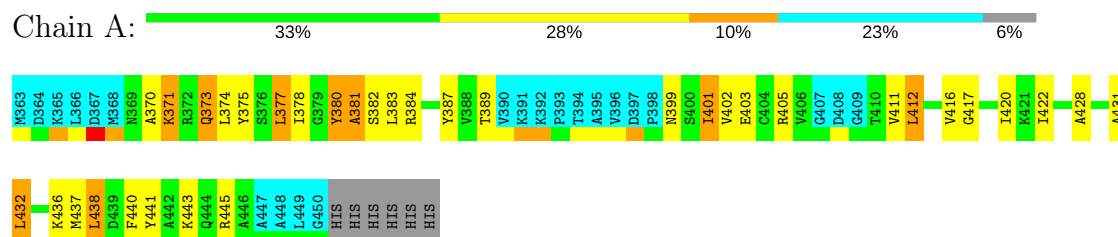
4.2.6 Score per residue for model 6

- Molecule 1: Ribonuclease III



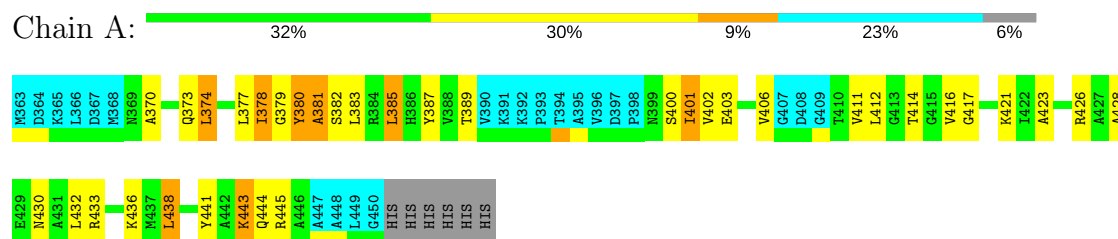
4.2.7 Score per residue for model 7

- Molecule 1: Ribonuclease III



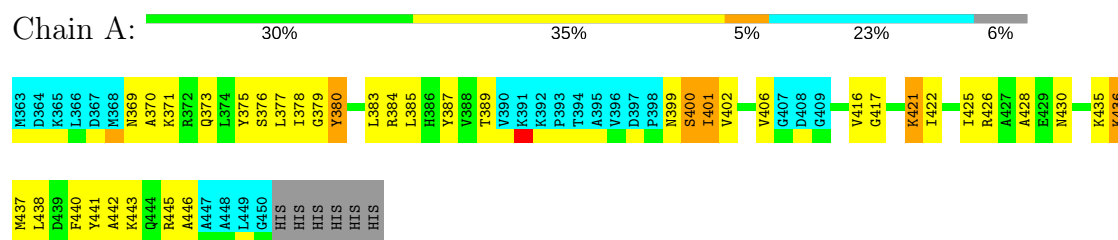
4.2.8 Score per residue for model 8

- Molecule 1: Ribonuclease III



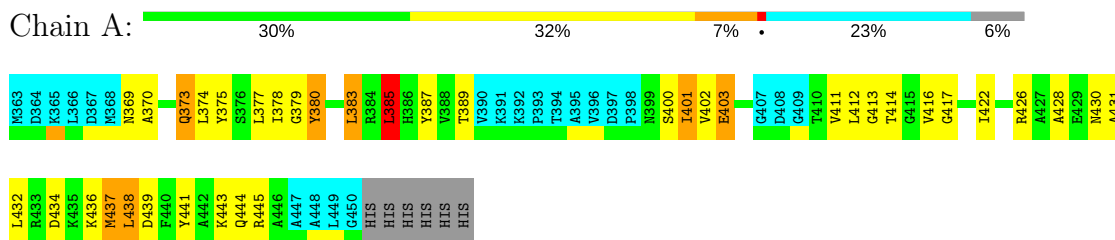
4.2.9 Score per residue for model 9

- Molecule 1: Ribonuclease III



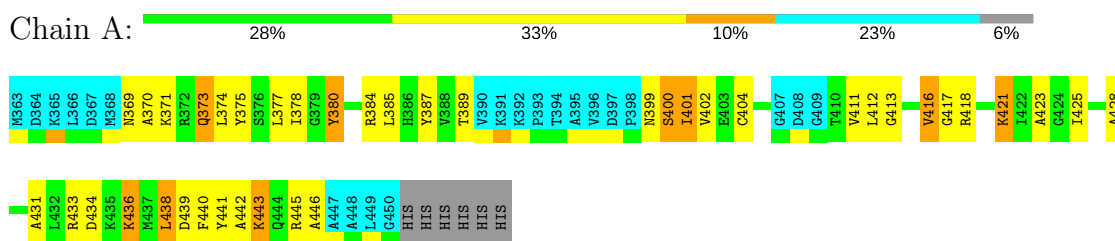
4.2.10 Score per residue for model 10

- Molecule 1: Ribonuclease III



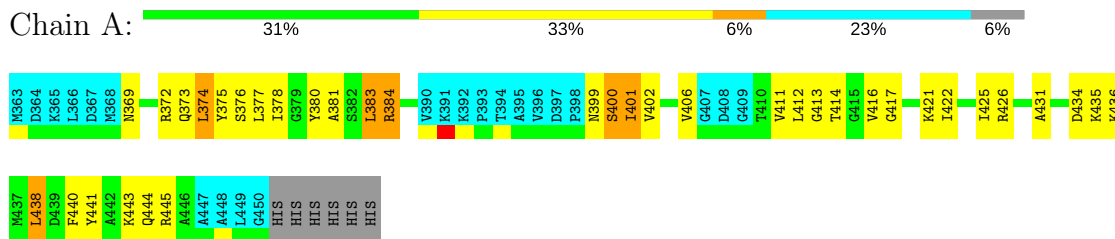
4.2.11 Score per residue for model 11

- Molecule 1: Ribonuclease III



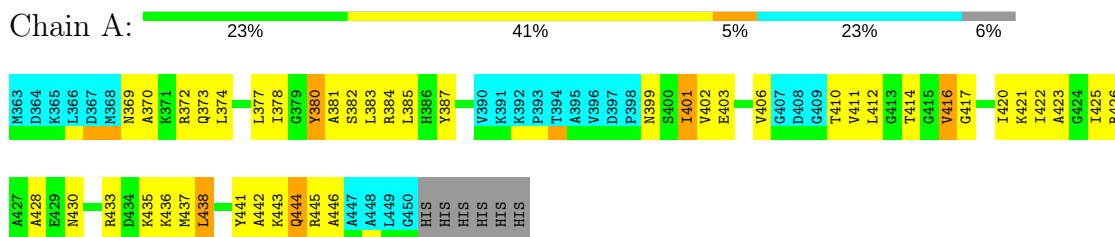
4.2.12 Score per residue for model 12

- Molecule 1: Ribonuclease III



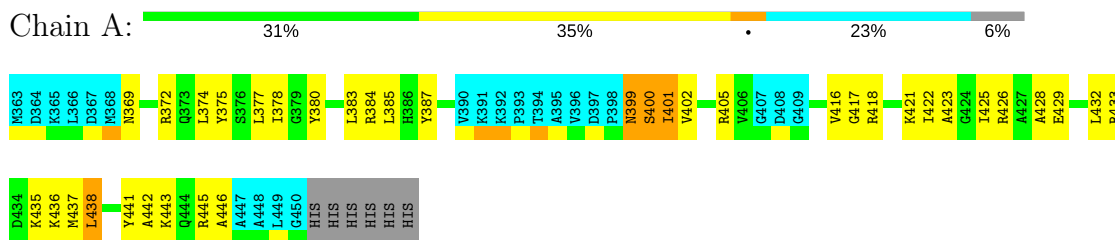
4.2.13 Score per residue for model 13

- Molecule 1: Ribonuclease III



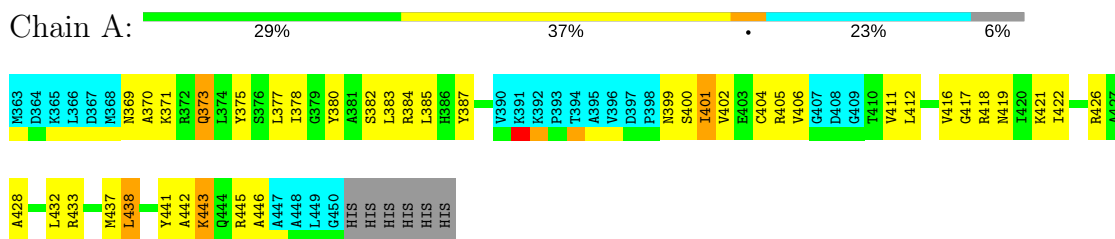
4.2.14 Score per residue for model 14

- Molecule 1: Ribonuclease III



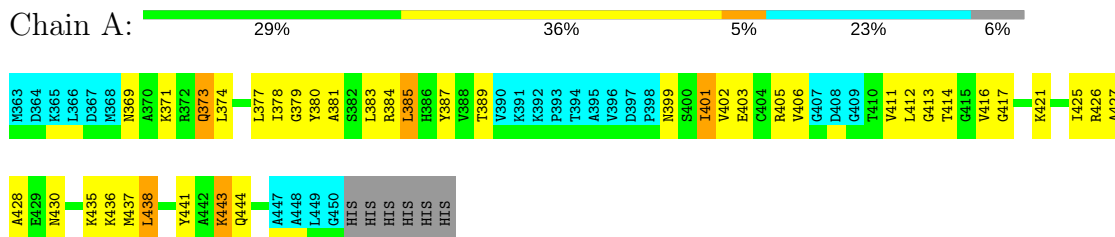
4.2.15 Score per residue for model 15

- Molecule 1: Ribonuclease III



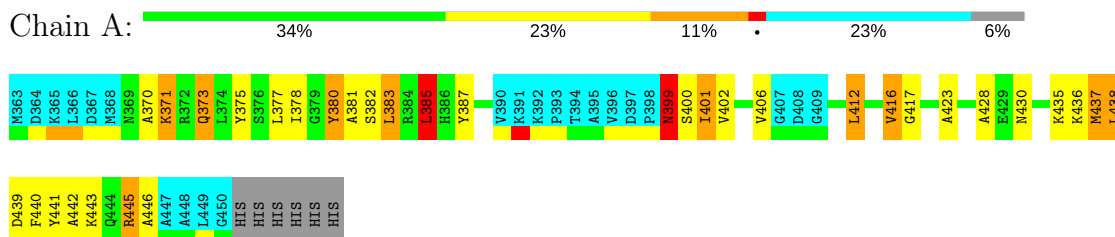
4.2.16 Score per residue for model 16

- Molecule 1: Ribonuclease III



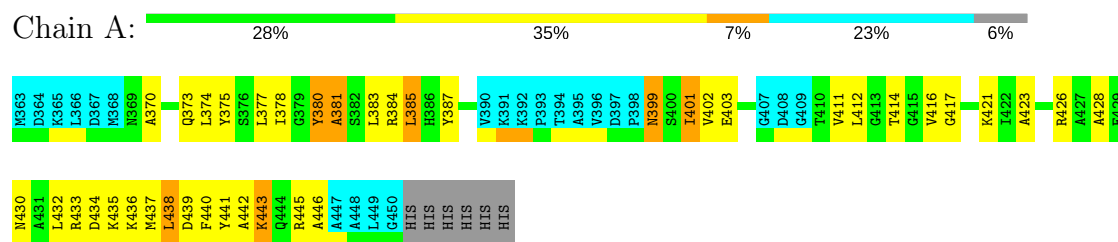
4.2.17 Score per residue for model 17

- Molecule 1: Ribonuclease III



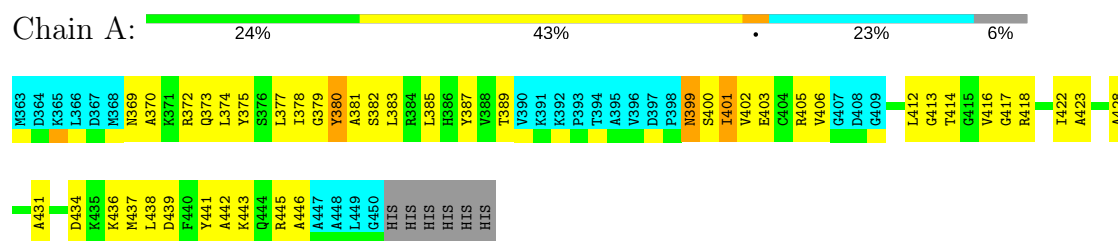
4.2.22 Score per residue for model 22

• Molecule 1: Ribonuclease III



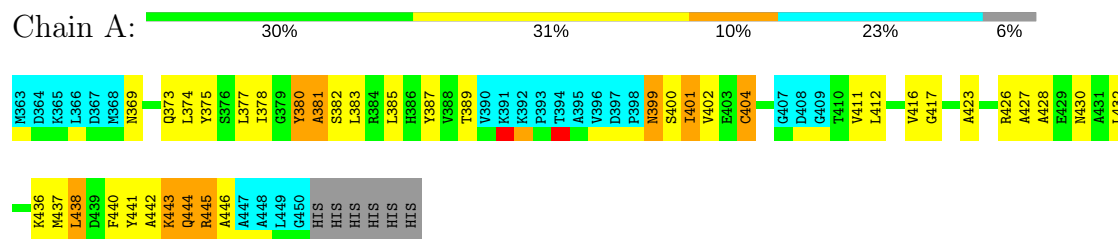
4.2.23 Score per residue for model 23

• Molecule 1: Ribonuclease III



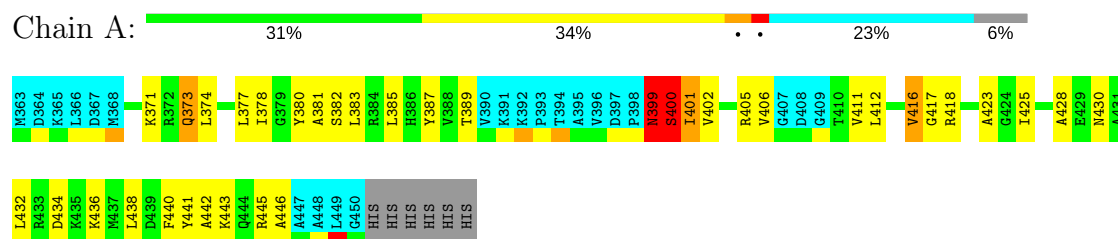
4.2.24 Score per residue for model 24

• Molecule 1: Ribonuclease III



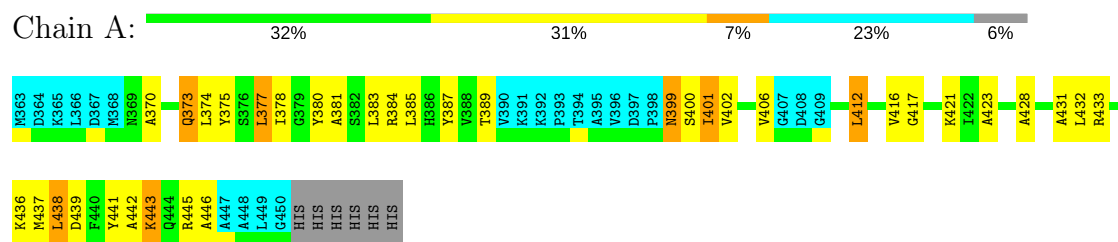
4.2.25 Score per residue for model 25

• Molecule 1: Ribonuclease III



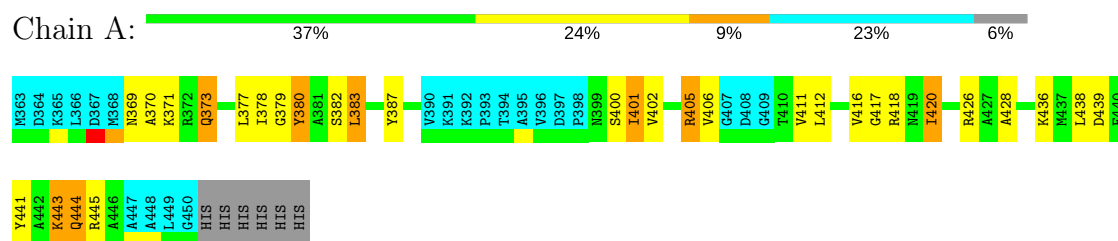
4.2.26 Score per residue for model 26

• Molecule 1: Ribonuclease III



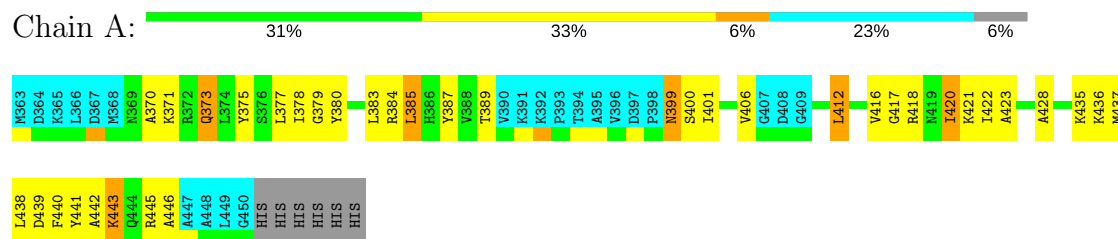
4.2.27 Score per residue for model 27

• Molecule 1: Ribonuclease III



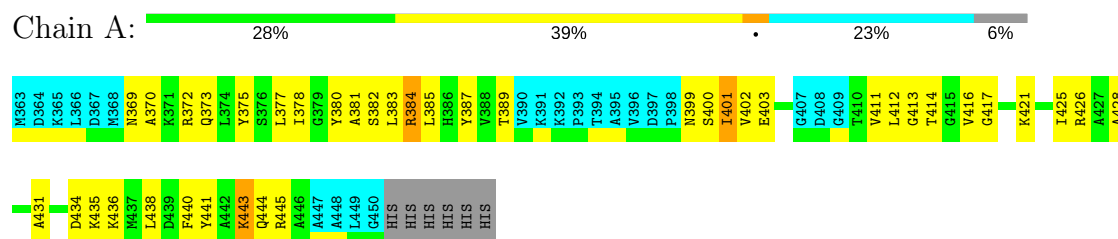
4.2.28 Score per residue for model 28

• Molecule 1: Ribonuclease III



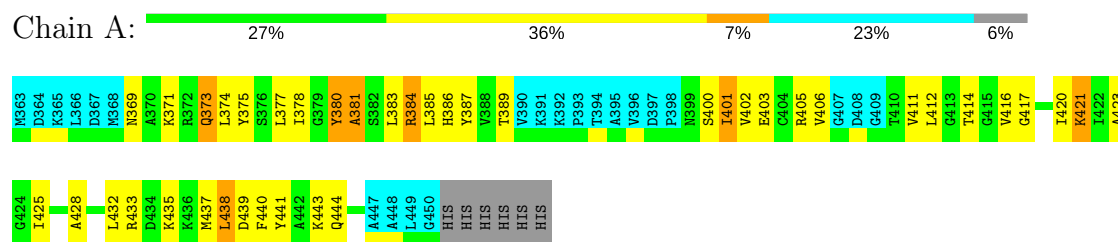
4.2.29 Score per residue for model 29

• Molecule 1: Ribonuclease III



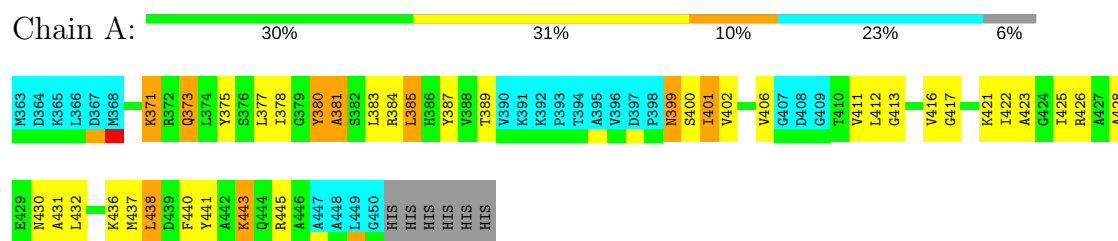
4.2.30 Score per residue for model 30

- Molecule 1: Ribonuclease III



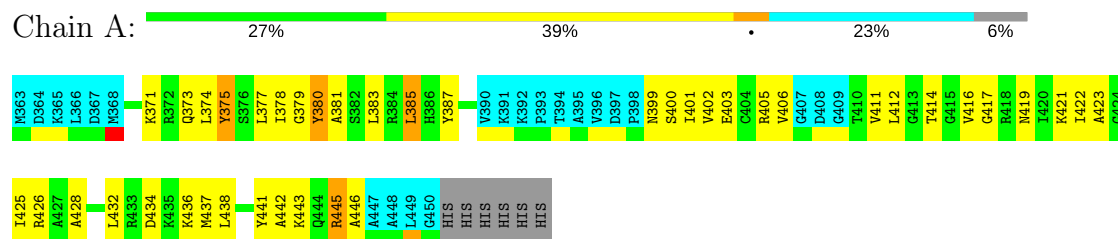
4.2.31 Score per residue for model 31

- Molecule 1: Ribonuclease III



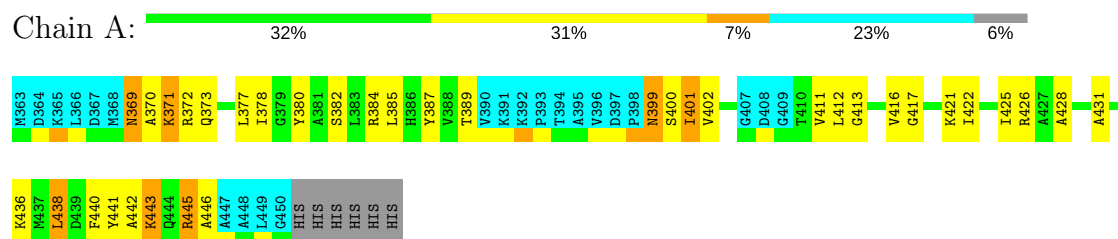
4.2.32 Score per residue for model 32

- Molecule 1: Ribonuclease III



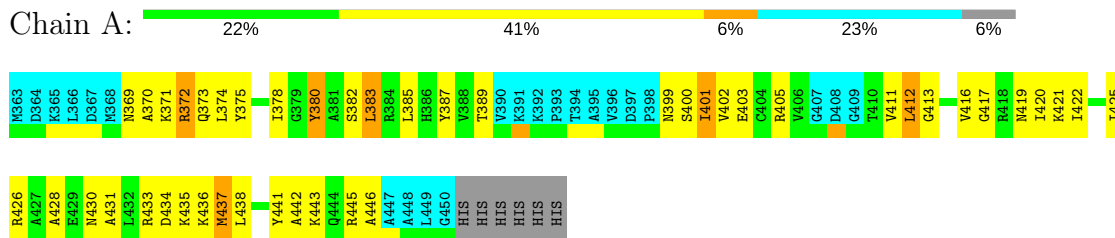
4.2.33 Score per residue for model 33

- Molecule 1: Ribonuclease III



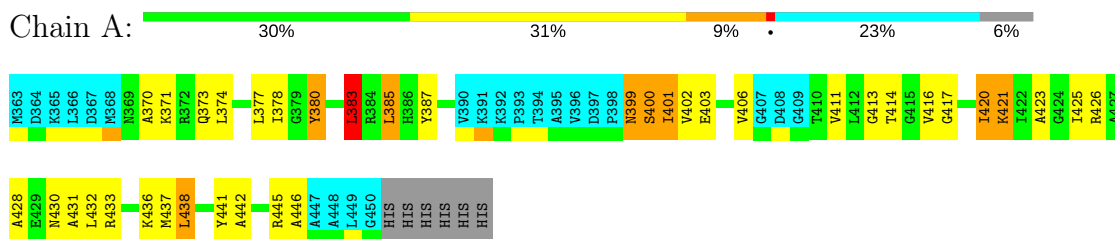
4.2.34 Score per residue for model 34

- Molecule 1: Ribonuclease III



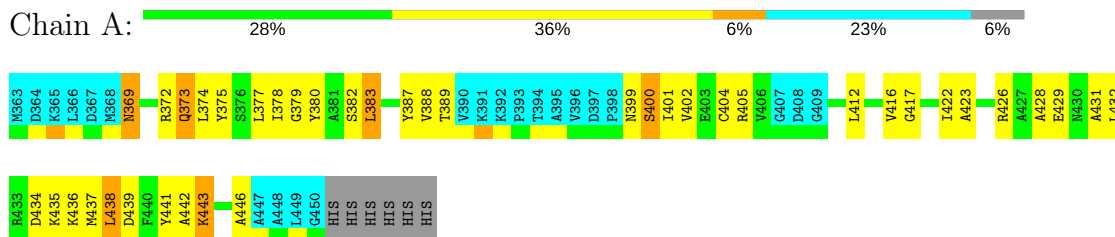
4.2.35 Score per residue for model 35

- Molecule 1: Ribonuclease III



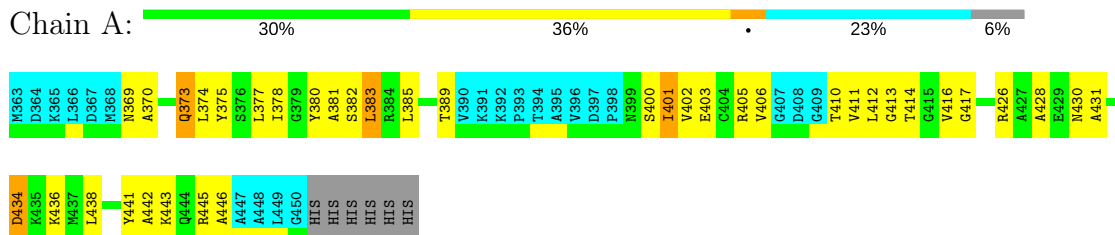
4.2.36 Score per residue for model 36

- Molecule 1: Ribonuclease III



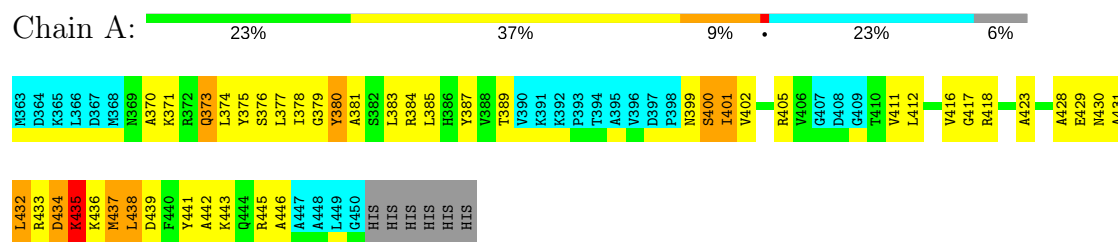
4.2.37 Score per residue for model 37

- Molecule 1: Ribonuclease III



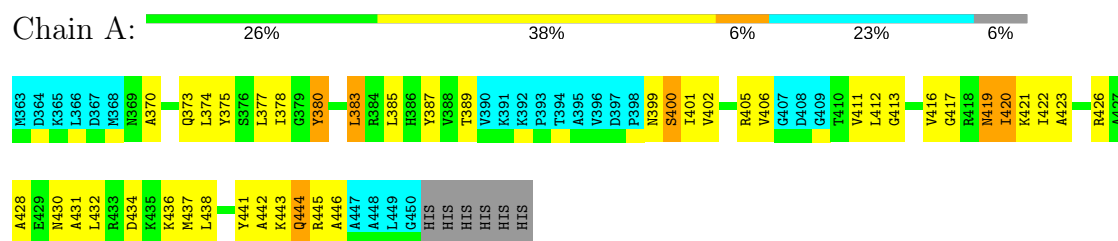
4.2.38 Score per residue for model 38

• Molecule 1: Ribonuclease III



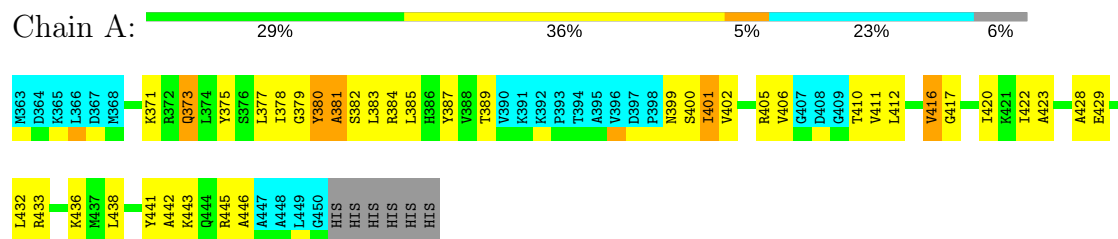
4.2.39 Score per residue for model 39

• Molecule 1: Ribonuclease III



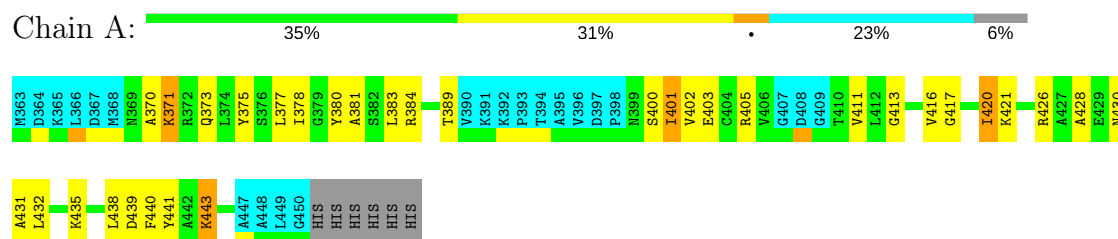
4.2.40 Score per residue for model 40

• Molecule 1: Ribonuclease III



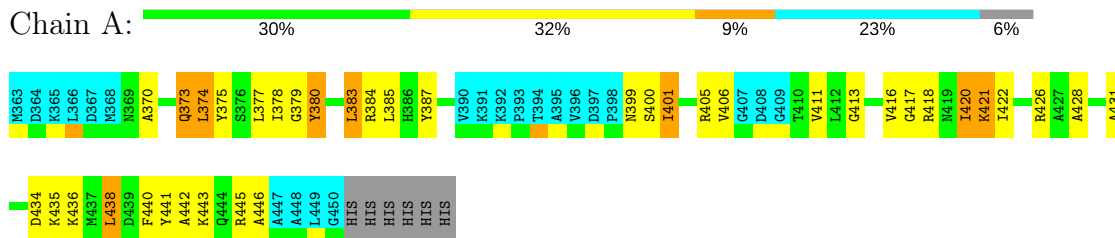
4.2.41 Score per residue for model 41

• Molecule 1: Ribonuclease III



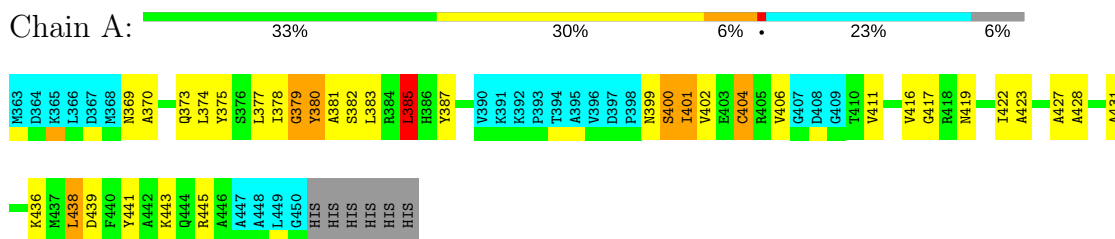
4.2.42 Score per residue for model 42

- Molecule 1: Ribonuclease III



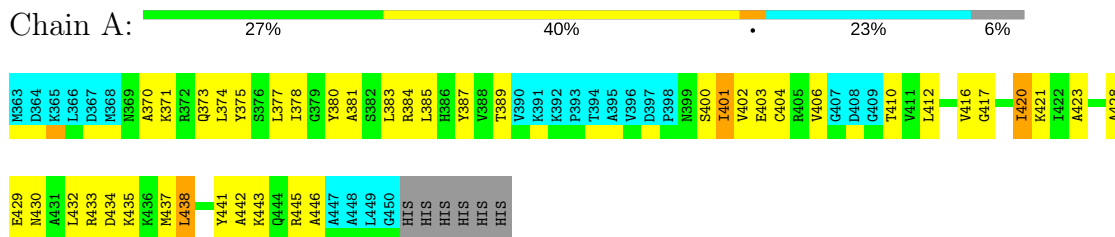
4.2.43 Score per residue for model 43

- Molecule 1: Ribonuclease III



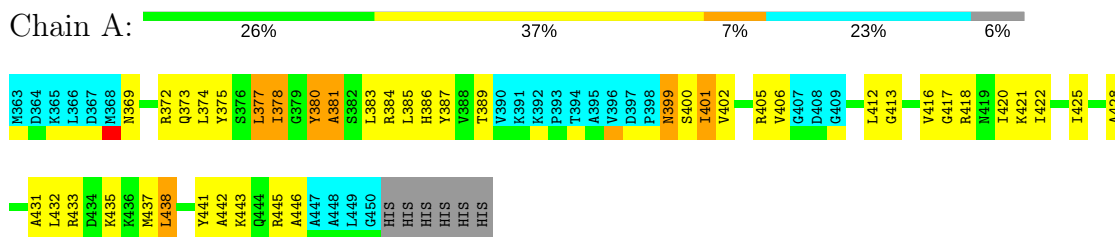
4.2.44 Score per residue for model 44

- Molecule 1: Ribonuclease III



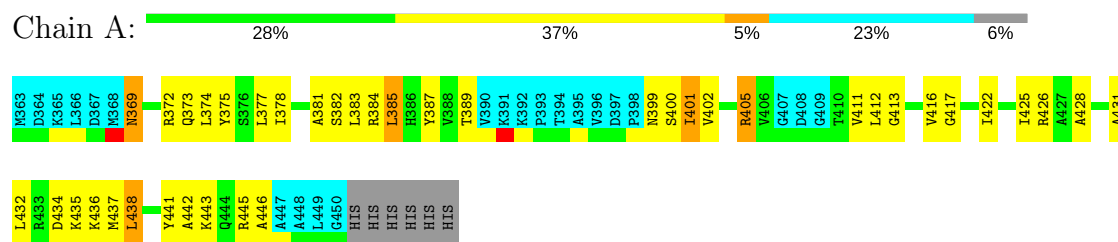
4.2.45 Score per residue for model 45

- Molecule 1: Ribonuclease III



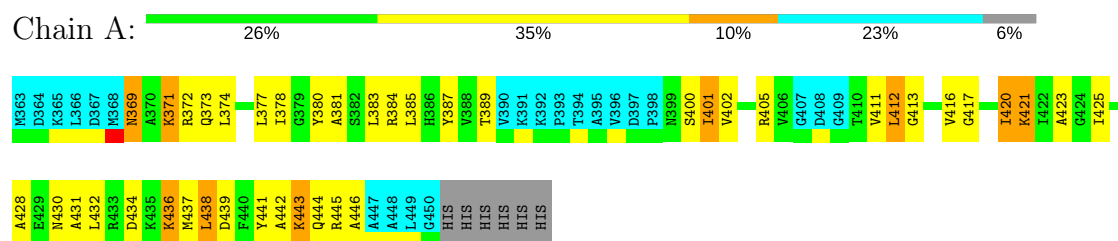
4.2.46 Score per residue for model 46

- Molecule 1: Ribonuclease III



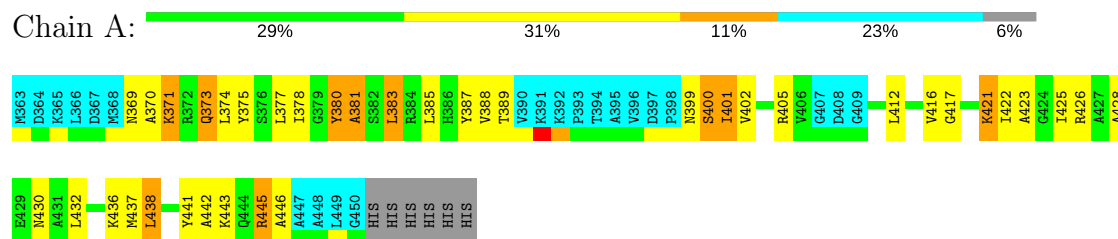
4.2.47 Score per residue for model 47 (medoid)

- Molecule 1: Ribonuclease III



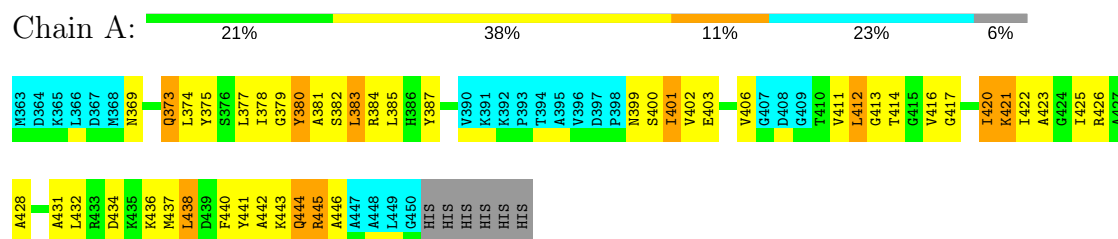
4.2.48 Score per residue for model 48

- Molecule 1: Ribonuclease III



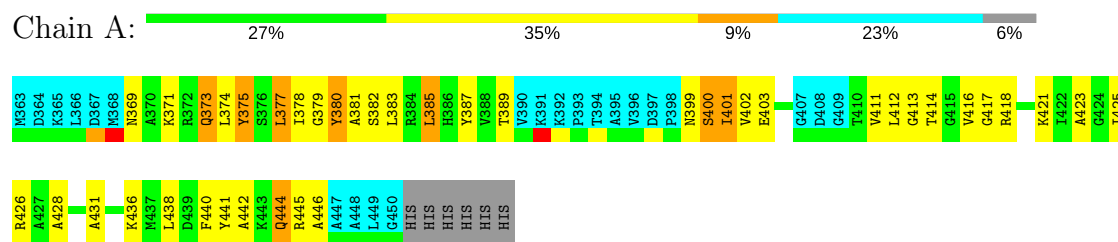
4.2.49 Score per residue for model 49

- Molecule 1: Ribonuclease III



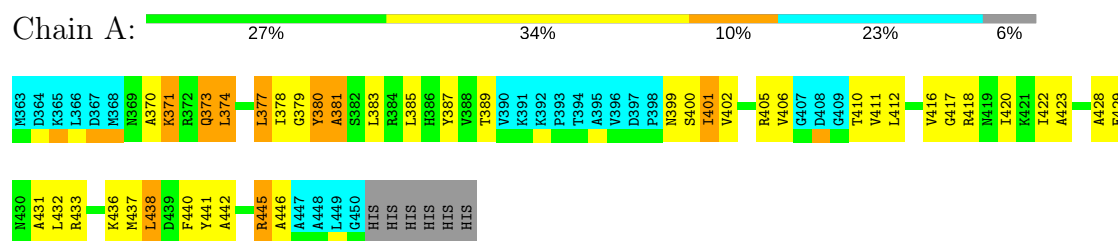
4.2.50 Score per residue for model 50

• Molecule 1: Ribonuclease III



4.2.51 Score per residue for model 51

• Molecule 1: Ribonuclease III



5 Refinement protocol and experimental data overview

Of the 51 calculated structures, 51 were deposited, based on the following criterion: *STRUCTURES WITH ACCEPTABLE COVALENT GEOMETRY*.

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

Software name	Classification	Version
CNS	refinement	
SPARKY	structure solution	
CNS	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	519	537	550	27±6
All	All	26469	27387	28050	1385

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:383:LEU:HD21	1:A:406:VAL:HG12	0.91	1.42	13	5
1:A:442:ALA:O	1:A:446:ALA:HB3	0.89	1.67	51	38
1:A:383:LEU:HD11	1:A:441:TYR:CE2	0.88	2.03	36	12
1:A:377:LEU:HD23	1:A:377:LEU:C	0.85	1.92	26	1
1:A:377:LEU:HD23	1:A:378:ILE:N	0.84	1.86	26	1
1:A:374:LEU:HD13	1:A:432:LEU:HD22	0.83	1.50	25	1
1:A:383:LEU:HD12	1:A:441:TYR:CE2	0.83	2.08	32	5
1:A:389:THR:HG21	1:A:420:ILE:HD12	0.82	1.48	39	5
1:A:370:ALA:HB1	1:A:428:ALA:HB3	0.81	1.52	13	29
1:A:377:LEU:CD1	1:A:378:ILE:HG23	0.79	2.07	50	2
1:A:389:THR:HG21	1:A:420:ILE:CD1	0.79	2.07	39	5
1:A:383:LEU:HD22	1:A:441:TYR:CE2	0.79	2.12	3	17
1:A:421:LYS:O	1:A:425:ILE:HD12	0.78	1.79	13	9
1:A:374:LEU:HD13	1:A:432:LEU:HD12	0.78	1.52	24	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:374:LEU:HD11	1:A:431:ALA:HB3	0.78	1.53	12	8
1:A:374:LEU:HD23	1:A:385:LEU:HD11	0.77	1.55	47	15
1:A:383:LEU:HD22	1:A:441:TYR:CE1	0.77	2.14	8	1
1:A:378:ILE:HD12	1:A:383:LEU:HD11	0.77	1.55	5	4
1:A:389:THR:CB	1:A:402:VAL:HG22	0.77	2.10	20	8
1:A:383:LEU:HD11	1:A:441:TYR:CE1	0.76	2.15	19	1
1:A:377:LEU:HD23	1:A:438:LEU:HD21	0.76	1.55	32	1
1:A:401:ILE:HG12	1:A:416:VAL:HG22	0.74	1.59	19	25
1:A:373:GLN:NE2	1:A:377:LEU:HD22	0.73	1.98	49	16
1:A:378:ILE:HD12	1:A:383:LEU:CD2	0.73	2.12	38	10
1:A:383:LEU:HD11	1:A:406:VAL:HG21	0.73	1.58	8	1
1:A:389:THR:HA	1:A:402:VAL:HG22	0.73	1.61	33	8
1:A:374:LEU:HD21	1:A:431:ALA:CB	0.73	2.13	26	4
1:A:383:LEU:HD11	1:A:441:TYR:CD2	0.72	2.19	50	7
1:A:389:THR:HG23	1:A:402:VAL:CG2	0.72	2.14	20	8
1:A:374:LEU:HA	1:A:377:LEU:HD22	0.72	1.60	26	1
1:A:373:GLN:OE1	1:A:432:LEU:HD11	0.71	1.84	8	2
1:A:405:ARG:HG3	1:A:411:VAL:HG22	0.71	1.59	27	5
1:A:441:TYR:CD2	1:A:445:ARG:NH1	0.71	2.58	48	1
1:A:380:TYR:CE2	1:A:445:ARG:NE	0.71	2.59	18	2
1:A:389:THR:HG23	1:A:402:VAL:HG22	0.70	1.64	34	8
1:A:401:ILE:HD13	1:A:402:VAL:N	0.70	2.02	25	31
1:A:374:LEU:HD23	1:A:385:LEU:CD1	0.70	2.17	1	7
1:A:389:THR:HG22	1:A:402:VAL:HG22	0.69	1.61	16	21
1:A:405:ARG:HG2	1:A:411:VAL:HG22	0.69	1.64	51	10
1:A:377:LEU:CD2	1:A:378:ILE:HG23	0.68	2.19	26	1
1:A:378:ILE:HD12	1:A:383:LEU:HD21	0.67	1.66	29	6
1:A:373:GLN:NE2	1:A:432:LEU:HD22	0.66	2.05	18	4
1:A:441:TYR:O	1:A:445:ARG:HG2	0.66	1.91	48	2
1:A:434:ASP:O	1:A:436:LYS:N	0.66	2.29	38	1
1:A:406:VAL:HG22	1:A:410:THR:O	0.66	1.91	21	7
1:A:385:LEU:O	1:A:385:LEU:HD23	0.66	1.91	13	10
1:A:389:THR:CA	1:A:402:VAL:HG22	0.66	2.21	33	8
1:A:380:TYR:HB3	1:A:445:ARG:HB3	0.66	1.68	48	1
1:A:389:THR:CG2	1:A:402:VAL:HG22	0.65	2.21	34	8
1:A:371:LYS:HG2	1:A:385:LEU:HD21	0.65	1.68	20	8
1:A:380:TYR:CE1	1:A:383:LEU:HD23	0.65	2.27	35	3
1:A:380:TYR:CE2	1:A:445:ARG:CZ	0.65	2.80	48	2
1:A:413:GLY:O	1:A:427:ALA:HB1	0.65	1.90	16	3
1:A:387:TYR:OH	1:A:428:ALA:HB2	0.65	1.91	22	46
1:A:405:ARG:CG	1:A:411:VAL:HG22	0.65	2.22	16	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:383:LEU:CD2	1:A:406:VAL:HG12	0.65	2.22	5	5
1:A:377:LEU:HD12	1:A:378:ILE:HG23	0.65	1.69	7	2
1:A:377:LEU:HD23	1:A:378:ILE:HG23	0.64	1.70	26	1
1:A:445:ARG:N	1:A:445:ARG:CD	0.64	2.61	51	1
1:A:385:LEU:HA	1:A:406:VAL:HG12	0.64	1.68	9	7
1:A:438:LEU:HD13	1:A:438:LEU:O	0.63	1.93	50	16
1:A:385:LEU:HD23	1:A:385:LEU:O	0.63	1.94	9	3
1:A:377:LEU:CD1	1:A:438:LEU:HD11	0.63	2.24	7	2
1:A:383:LEU:HD11	1:A:441:TYR:CD1	0.63	2.28	19	1
1:A:373:GLN:NE2	1:A:377:LEU:HD13	0.63	2.08	45	10
1:A:389:THR:HG22	1:A:402:VAL:CG2	0.62	2.24	50	3
1:A:441:TYR:C	1:A:445:ARG:HG2	0.62	2.15	18	2
1:A:402:VAL:HG23	1:A:423:ALA:HB1	0.62	1.71	39	17
1:A:374:LEU:HD13	1:A:432:LEU:CD1	0.62	2.25	2	5
1:A:383:LEU:HD12	1:A:441:TYR:CD2	0.61	2.30	5	3
1:A:416:VAL:HG22	1:A:417:GLY:H	0.61	1.56	49	24
1:A:373:GLN:O	1:A:377:LEU:HB3	0.61	1.96	26	1
1:A:377:LEU:HB3	1:A:438:LEU:HD11	0.61	1.71	11	28
1:A:378:ILE:HG22	1:A:441:TYR:CB	0.61	2.25	12	45
1:A:378:ILE:HG21	1:A:438:LEU:HD22	0.61	1.72	48	2
1:A:377:LEU:CD2	1:A:377:LEU:C	0.61	2.69	26	1
1:A:370:ALA:HB1	1:A:428:ALA:CB	0.60	2.27	44	20
1:A:413:GLY:HA3	1:A:431:ALA:HB2	0.60	1.72	20	18
1:A:373:GLN:O	1:A:377:LEU:HD13	0.60	1.97	16	2
1:A:445:ARG:HD2	1:A:445:ARG:N	0.60	2.11	51	2
1:A:429:GLU:HA	1:A:432:LEU:HD12	0.60	1.74	44	4
1:A:371:LYS:HG3	1:A:385:LEU:HD21	0.60	1.73	32	3
1:A:377:LEU:HD13	1:A:438:LEU:HD11	0.60	1.73	7	2
1:A:373:GLN:C	1:A:377:LEU:HD23	0.59	2.17	50	2
1:A:374:LEU:HD13	1:A:432:LEU:HG	0.59	1.72	47	6
1:A:400:SER:O	1:A:423:ALA:HB2	0.59	1.98	6	24
1:A:378:ILE:HD12	1:A:383:LEU:CD1	0.59	2.27	13	2
1:A:428:ALA:O	1:A:432:LEU:HD13	0.59	1.98	21	6
1:A:445:ARG:CD	1:A:445:ARG:H	0.59	2.10	18	1
1:A:445:ARG:CZ	1:A:446:ALA:HB2	0.59	2.27	24	3
1:A:378:ILE:HG22	1:A:441:TYR:HB2	0.58	1.75	39	42
1:A:420:ILE:HD11	1:A:421:LYS:CE	0.58	2.29	42	1
1:A:373:GLN:HA	1:A:373:GLN:NE2	0.58	2.14	16	1
1:A:389:THR:HG21	1:A:420:ILE:HG22	0.58	1.74	6	1
1:A:438:LEU:O	1:A:438:LEU:HD13	0.58	1.99	33	10
1:A:383:LEU:HD13	1:A:406:VAL:CG1	0.58	2.29	37	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:373:GLN:HG2	1:A:432:LEU:HD21	0.58	1.75	22	2
1:A:399:ASN:N	1:A:416:VAL:HG21	0.58	2.14	25	1
1:A:380:TYR:CD2	1:A:445:ARG:HD2	0.58	2.34	18	2
1:A:442:ALA:O	1:A:446:ALA:CB	0.57	2.51	18	3
1:A:412:LEU:HD11	1:A:437:MET:SD	0.57	2.40	28	9
1:A:420:ILE:HD12	1:A:421:LYS:N	0.57	2.14	35	2
1:A:374:LEU:CD1	1:A:432:LEU:HD12	0.57	2.28	24	1
1:A:445:ARG:H	1:A:445:ARG:CD	0.57	2.11	51	1
1:A:416:VAL:HG13	1:A:417:GLY:N	0.57	2.14	17	2
1:A:374:LEU:HD21	1:A:431:ALA:HB3	0.57	1.76	26	3
1:A:377:LEU:HD11	1:A:378:ILE:HG23	0.57	1.75	50	2
1:A:378:ILE:HB	1:A:441:TYR:CD2	0.56	2.35	51	3
1:A:378:ILE:O	1:A:383:LEU:HD12	0.56	1.99	43	6
1:A:373:GLN:CG	1:A:432:LEU:HD21	0.56	2.30	22	2
1:A:374:LEU:HD13	1:A:432:LEU:CD2	0.56	2.29	25	1
1:A:383:LEU:HD13	1:A:441:TYR:CE2	0.56	2.35	23	7
1:A:445:ARG:CD	1:A:445:ARG:N	0.56	2.69	18	1
1:A:441:TYR:CD2	1:A:445:ARG:NE	0.56	2.73	51	2
1:A:383:LEU:HD11	1:A:406:VAL:HG11	0.56	1.77	30	6
1:A:441:TYR:CD2	1:A:445:ARG:CZ	0.55	2.90	48	3
1:A:380:TYR:CE2	1:A:445:ARG:NH1	0.55	2.74	48	1
1:A:370:ALA:CB	1:A:428:ALA:HB3	0.55	2.31	13	1
1:A:404:CYS:SG	1:A:427:ALA:HB1	0.55	2.41	19	3
1:A:383:LEU:HD12	1:A:406:VAL:HB	0.55	1.78	26	1
1:A:377:LEU:HG	1:A:438:LEU:HD11	0.54	1.79	26	1
1:A:383:LEU:HD21	1:A:406:VAL:CG1	0.54	2.28	13	1
1:A:411:VAL:HG21	1:A:414:THR:OG1	0.53	2.04	6	6
1:A:373:GLN:HE22	1:A:377:LEU:HD22	0.53	1.63	40	5
1:A:420:ILE:HD11	1:A:421:LYS:HE2	0.53	1.79	42	1
1:A:373:GLN:OE1	1:A:377:LEU:HD22	0.53	2.02	5	1
1:A:380:TYR:O	1:A:381:ALA:HB2	0.53	2.03	18	12
1:A:384:ARG:CG	1:A:384:ARG:O	0.53	2.57	40	1
1:A:401:ILE:HG12	1:A:416:VAL:HG23	0.53	1.80	11	4
1:A:403:GLU:HG2	1:A:414:THR:HG23	0.53	1.80	32	12
1:A:399:ASN:HB2	1:A:416:VAL:HG21	0.52	1.81	36	2
1:A:416:VAL:HG22	1:A:417:GLY:N	0.52	2.19	34	12
1:A:374:LEU:HD11	1:A:432:LEU:HD12	0.52	1.81	7	1
1:A:389:THR:HG21	1:A:420:ILE:HG23	0.52	1.80	19	2
1:A:441:TYR:CE2	1:A:445:ARG:NH2	0.52	2.77	18	2
1:A:421:LYS:HD3	1:A:425:ILE:HD11	0.52	1.81	30	3
1:A:373:GLN:O	1:A:377:LEU:HD23	0.52	2.05	50	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:420:ILE:HD12	1:A:421:LYS:H	0.52	1.65	35	2
1:A:420:ILE:N	1:A:420:ILE:HD13	0.52	2.20	41	5
1:A:374:LEU:HD11	1:A:431:ALA:CB	0.52	2.32	12	1
1:A:437:MET:HE2	1:A:441:TYR:CD1	0.52	2.40	38	1
1:A:375:TYR:CD2	1:A:385:LEU:HD22	0.52	2.40	50	2
1:A:441:TYR:O	1:A:445:ARG:HD3	0.51	2.05	51	2
1:A:420:ILE:HD13	1:A:420:ILE:N	0.51	2.20	42	1
1:A:383:LEU:HD22	1:A:441:TYR:CD2	0.51	2.41	7	4
1:A:388:VAL:HG21	1:A:405:ARG:NE	0.51	2.19	48	1
1:A:416:VAL:HG12	1:A:417:GLY:N	0.51	2.21	15	25
1:A:380:TYR:CD2	1:A:445:ARG:CD	0.51	2.94	18	2
1:A:373:GLN:OE1	1:A:377:LEU:HD13	0.51	2.05	42	6
1:A:413:GLY:CA	1:A:431:ALA:HB2	0.51	2.36	35	6
1:A:374:LEU:HD11	1:A:432:LEU:HA	0.51	1.82	38	1
1:A:389:THR:OG1	1:A:402:VAL:HG22	0.51	2.06	20	5
1:A:383:LEU:CD1	1:A:406:VAL:HG11	0.51	2.36	12	2
1:A:388:VAL:HG21	1:A:405:ARG:CZ	0.50	2.36	48	1
1:A:441:TYR:O	1:A:445:ARG:N	0.50	2.42	18	2
1:A:380:TYR:O	1:A:381:ALA:HB3	0.50	2.07	17	6
1:A:373:GLN:NE2	1:A:373:GLN:HA	0.50	2.21	7	1
1:A:371:LYS:HE3	1:A:385:LEU:HD23	0.50	1.83	31	1
1:A:399:ASN:ND2	1:A:416:VAL:HG13	0.50	2.22	9	1
1:A:383:LEU:CD1	1:A:441:TYR:CE1	0.50	2.93	19	2
1:A:374:LEU:HD11	1:A:432:LEU:CD1	0.50	2.37	7	1
1:A:374:LEU:O	1:A:378:ILE:CG1	0.49	2.60	50	5
1:A:389:THR:CG2	1:A:402:VAL:CG2	0.49	2.89	6	8
1:A:402:VAL:HG23	1:A:423:ALA:CB	0.49	2.37	5	5
1:A:373:GLN:NE2	1:A:377:LEU:CD1	0.49	2.76	16	6
1:A:383:LEU:HD13	1:A:406:VAL:HG11	0.49	1.85	37	2
1:A:369:ASN:HA	1:A:372:ARG:HG2	0.48	1.84	34	1
1:A:383:LEU:HD22	1:A:406:VAL:HG11	0.48	1.85	25	3
1:A:422:ILE:HD12	1:A:422:ILE:N	0.48	2.24	43	10
1:A:383:LEU:HD11	1:A:406:VAL:CG2	0.48	2.37	8	1
1:A:389:THR:OG1	1:A:402:VAL:CG2	0.48	2.62	20	8
1:A:383:LEU:CD1	1:A:441:TYR:CE2	0.48	2.94	43	7
1:A:380:TYR:CE2	1:A:445:ARG:CD	0.48	2.97	18	2
1:A:383:LEU:HD22	1:A:441:TYR:CD1	0.48	2.44	8	1
1:A:422:ILE:HA	1:A:425:ILE:HD12	0.47	1.84	45	2
1:A:441:TYR:HA	1:A:445:ARG:HD3	0.47	1.85	51	2
1:A:371:LYS:CG	1:A:385:LEU:HD21	0.47	2.40	40	2
1:A:374:LEU:CD1	1:A:438:LEU:HD21	0.47	2.40	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:401:ILE:HD12	1:A:403:GLU:OE2	0.47	2.09	10	1
1:A:373:GLN:CD	1:A:432:LEU:HD11	0.47	2.30	8	1
1:A:403:GLU:HG3	1:A:414:THR:HG23	0.47	1.87	10	3
1:A:385:LEU:C	1:A:385:LEU:HD23	0.47	2.28	3	2
1:A:374:LEU:HB3	1:A:385:LEU:HD13	0.47	1.85	8	2
1:A:374:LEU:HD12	1:A:432:LEU:HD21	0.47	1.85	5	1
1:A:378:ILE:O	1:A:445:ARG:HG3	0.47	2.10	51	2
1:A:411:VAL:HG13	1:A:411:VAL:O	0.47	2.10	49	10
1:A:377:LEU:C	1:A:377:LEU:HD12	0.47	2.30	7	2
1:A:378:ILE:CG2	1:A:438:LEU:HD12	0.47	2.40	32	2
1:A:383:LEU:HD13	1:A:441:TYR:OH	0.47	2.10	7	2
1:A:412:LEU:HD23	1:A:431:ALA:O	0.46	2.10	38	1
1:A:383:LEU:CD2	1:A:441:TYR:CE2	0.46	2.99	40	4
1:A:380:TYR:CE2	1:A:445:ARG:HD2	0.46	2.45	18	2
1:A:373:GLN:HE21	1:A:377:LEU:HD22	0.46	1.70	35	3
1:A:422:ILE:N	1:A:422:ILE:HD12	0.46	2.26	4	13
1:A:411:VAL:O	1:A:411:VAL:HG13	0.46	2.11	22	10
1:A:378:ILE:HG13	1:A:379:GLY:N	0.46	2.26	51	16
1:A:378:ILE:O	1:A:445:ARG:HD2	0.46	2.11	48	1
1:A:378:ILE:HG22	1:A:441:TYR:HB3	0.46	1.87	25	12
1:A:383:LEU:HD23	1:A:406:VAL:HB	0.46	1.86	25	1
1:A:385:LEU:HD23	1:A:385:LEU:C	0.46	2.29	9	1
1:A:378:ILE:O	1:A:445:ARG:CD	0.46	2.64	48	1
1:A:380:TYR:HE1	1:A:383:LEU:HD23	0.46	1.69	35	2
1:A:387:TYR:OH	1:A:428:ALA:HA	0.46	2.11	38	1
1:A:378:ILE:HA	1:A:445:ARG:HG3	0.46	1.88	48	2
1:A:435:LYS:O	1:A:439:ASP:N	0.45	2.48	38	1
1:A:374:LEU:HD12	1:A:378:ILE:CD1	0.45	2.41	8	1
1:A:377:LEU:HD23	1:A:438:LEU:HD11	0.45	1.87	18	3
1:A:373:GLN:NE2	1:A:432:LEU:HD21	0.45	2.25	49	1
1:A:380:TYR:CE2	1:A:444:GLN:HG2	0.45	2.47	24	5
1:A:421:LYS:NZ	1:A:425:ILE:HD11	0.45	2.26	16	1
1:A:436:LYS:HD2	1:A:436:LYS:N	0.45	2.27	48	1
1:A:441:TYR:CE2	1:A:445:ARG:NH1	0.45	2.84	48	1
1:A:402:VAL:HG12	1:A:403:GLU:N	0.45	2.27	34	6
1:A:378:ILE:CG2	1:A:438:LEU:CD1	0.45	2.95	32	3
1:A:401:ILE:CG1	1:A:416:VAL:HG22	0.45	2.39	23	1
1:A:389:THR:HG22	1:A:402:VAL:CG1	0.44	2.41	19	1
1:A:378:ILE:CG2	1:A:441:TYR:CB	0.44	2.95	2	32
1:A:380:TYR:CE1	1:A:383:LEU:CD2	0.44	2.99	27	2
1:A:400:SER:O	1:A:423:ALA:CB	0.44	2.65	25	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:441:TYR:HB3	1:A:445:ARG:CG	0.44	2.42	18	1
1:A:445:ARG:HG3	1:A:446:ALA:N	0.44	2.27	49	2
1:A:412:LEU:CD2	1:A:431:ALA:O	0.44	2.65	38	1
1:A:420:ILE:HD11	1:A:421:LYS:HD2	0.44	1.89	49	1
1:A:399:ASN:HB3	1:A:416:VAL:CG2	0.44	2.43	28	1
1:A:429:GLU:O	1:A:432:LEU:HB2	0.44	2.13	38	1
1:A:378:ILE:HG21	1:A:438:LEU:CD2	0.44	2.41	48	2
1:A:377:LEU:CG	1:A:438:LEU:HD11	0.44	2.42	26	1
1:A:380:TYR:CD2	1:A:445:ARG:HD3	0.44	2.48	48	1
1:A:378:ILE:HA	1:A:445:ARG:HD2	0.44	1.88	48	1
1:A:441:TYR:CA	1:A:445:ARG:NE	0.43	2.81	48	1
1:A:400:SER:N	1:A:417:GLY:O	0.43	2.50	24	1
1:A:399:ASN:HB2	1:A:416:VAL:CG2	0.43	2.43	36	1
1:A:377:LEU:CD2	1:A:378:ILE:HG12	0.43	2.43	26	1
1:A:377:LEU:CD2	1:A:378:ILE:N	0.43	2.71	26	1
1:A:376:SER:C	1:A:377:LEU:HD12	0.43	2.34	38	1
1:A:434:ASP:C	1:A:436:LYS:N	0.43	2.69	38	1
1:A:418:ARG:CG	1:A:422:ILE:HD13	0.43	2.43	51	1
1:A:378:ILE:CG2	1:A:438:LEU:HD22	0.43	2.44	10	5
1:A:433:ARG:O	1:A:434:ASP:O	0.43	2.37	38	1
1:A:383:LEU:CD1	1:A:441:TYR:CD1	0.43	3.01	25	1
1:A:373:GLN:HG3	1:A:432:LEU:HD21	0.43	1.89	45	1
1:A:419:ASN:OD1	1:A:422:ILE:HD13	0.43	2.13	32	5
1:A:422:ILE:CD1	1:A:422:ILE:N	0.43	2.82	12	2
1:A:383:LEU:CD1	1:A:441:TYR:CD2	0.43	3.01	20	1
1:A:374:LEU:O	1:A:378:ILE:HG12	0.43	2.13	32	3
1:A:441:TYR:CA	1:A:445:ARG:HD3	0.43	2.44	18	2
1:A:436:LYS:N	1:A:436:LYS:CD	0.43	2.82	9	4
1:A:376:SER:O	1:A:377:LEU:HD12	0.43	2.14	9	1
1:A:412:LEU:HD11	1:A:437:MET:CG	0.43	2.44	28	3
1:A:380:TYR:HE2	1:A:445:ARG:CZ	0.42	2.24	48	1
1:A:431:ALA:O	1:A:438:LEU:HD23	0.42	2.14	35	1
1:A:399:ASN:ND2	1:A:399:ASN:N	0.42	2.67	3	3
1:A:387:TYR:OH	1:A:428:ALA:CB	0.42	2.67	50	10
1:A:445:ARG:NH1	1:A:446:ALA:HB2	0.42	2.29	24	1
1:A:378:ILE:CD1	1:A:412:LEU:HD22	0.42	2.43	49	2
1:A:378:ILE:CG2	1:A:438:LEU:HD13	0.42	2.45	38	1
1:A:380:TYR:OH	1:A:441:TYR:CE2	0.42	2.64	42	4
1:A:433:ARG:O	1:A:435:LYS:N	0.42	2.53	44	2
1:A:374:LEU:HD21	1:A:431:ALA:HB1	0.42	1.87	26	1
1:A:374:LEU:CA	1:A:377:LEU:HD22	0.42	2.36	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:401:ILE:O	1:A:401:ILE:CG2	0.42	2.68	19	3
1:A:378:ILE:O	1:A:380:TYR:CD2	0.42	2.73	23	3
1:A:374:LEU:CD1	1:A:432:LEU:CD1	0.42	2.97	7	1
1:A:373:GLN:HE21	1:A:432:LEU:HD21	0.42	1.74	31	1
1:A:369:ASN:O	1:A:372:ARG:CG	0.42	2.68	12	3
1:A:383:LEU:O	1:A:385:LEU:N	0.42	2.53	49	2
1:A:370:ALA:CB	1:A:428:ALA:CB	0.42	2.97	38	1
1:A:374:LEU:HD13	1:A:428:ALA:HB1	0.42	1.91	5	1
1:A:377:LEU:HD23	1:A:438:LEU:CD1	0.42	2.45	21	1
1:A:400:SER:O	1:A:417:GLY:N	0.42	2.53	24	2
1:A:399:ASN:OD1	1:A:416:VAL:CG1	0.42	2.68	23	4
1:A:373:GLN:CA	1:A:373:GLN:NE2	0.42	2.83	16	1
1:A:369:ASN:ND2	1:A:370:ALA:N	0.42	2.68	33	2
1:A:383:LEU:CD1	1:A:406:VAL:HG21	0.42	2.40	8	1
1:A:383:LEU:HD21	1:A:441:TYR:CE2	0.41	2.49	50	1
1:A:386:HIS:CD2	1:A:405:ARG:O	0.41	2.73	45	1
1:A:375:TYR:CD1	1:A:385:LEU:HB3	0.41	2.50	29	1
1:A:434:ASP:O	1:A:437:MET:N	0.41	2.54	38	1
1:A:373:GLN:NE2	1:A:377:LEU:CD2	0.41	2.83	9	3
1:A:378:ILE:CB	1:A:441:TYR:HB3	0.41	2.45	27	3
1:A:412:LEU:HD11	1:A:437:MET:HG2	0.41	1.92	32	1
1:A:434:ASP:O	1:A:435:LYS:C	0.41	2.58	38	1
1:A:380:TYR:CE2	1:A:444:GLN:CG	0.41	3.03	27	1
1:A:373:GLN:O	1:A:377:LEU:HB2	0.41	2.15	18	3
1:A:380:TYR:O	1:A:381:ALA:CB	0.41	2.68	18	1
1:A:399:ASN:N	1:A:399:ASN:ND2	0.41	2.68	14	1
1:A:399:ASN:HB3	1:A:416:VAL:HG21	0.41	1.92	28	1
1:A:388:VAL:CG2	1:A:405:ARG:CD	0.41	2.99	36	2
1:A:420:ILE:HD12	1:A:420:ILE:N	0.41	2.30	47	1
1:A:377:LEU:HD11	1:A:438:LEU:HD11	0.41	1.91	50	1
1:A:386:HIS:CD2	1:A:386:HIS:O	0.41	2.74	30	1
1:A:441:TYR:O	1:A:444:GLN:N	0.41	2.46	18	1
1:A:380:TYR:CD2	1:A:444:GLN:HG2	0.41	2.51	39	1
1:A:383:LEU:HD13	1:A:441:TYR:CE1	0.41	2.51	8	1
1:A:373:GLN:NE2	1:A:432:LEU:CD2	0.41	2.84	49	2
1:A:436:LYS:CD	1:A:436:LYS:N	0.41	2.84	11	1
1:A:420:ILE:H	1:A:420:ILE:HD12	0.40	1.76	3	1
1:A:371:LYS:HD3	1:A:385:LEU:HD23	0.40	1.92	18	1
1:A:383:LEU:HG	1:A:441:TYR:CE2	0.40	2.51	12	1
1:A:374:LEU:HG	1:A:378:ILE:HD11	0.40	1.93	35	1
1:A:416:VAL:CG1	1:A:417:GLY:N	0.40	2.85	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:374:LEU:HD12	1:A:432:LEU:CD2	0.40	2.47	44	1
1:A:374:LEU:HA	1:A:377:LEU:CD2	0.40	2.39	26	1
1:A:378:ILE:HD13	1:A:412:LEU:HD22	0.40	1.92	34	1
1:A:373:GLN:HG3	1:A:432:LEU:HD22	0.40	1.92	35	1
1:A:374:LEU:HD21	1:A:428:ALA:O	0.40	2.17	38	1
1:A:377:LEU:CD1	1:A:438:LEU:CD1	0.40	2.99	50	1
1:A:420:ILE:HD12	1:A:420:ILE:H	0.40	1.77	5	1
1:A:374:LEU:HA	1:A:377:LEU:HG	0.40	1.93	50	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	66/94 (70%)	56±2 (85±3%)	8±2 (12±3%)	2±1 (3±2%)	8	39
All	All	3366/4794 (70%)	2852 (85%)	404 (12%)	110 (3%)	8	39

All 11 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	381	ALA	32
1	A	434	ASP	19
1	A	384	ARG	18
1	A	385	LEU	14
1	A	369	ASN	10
1	A	379	GLY	6
1	A	383	LEU	4
1	A	378	ILE	3
1	A	399	ASN	2
1	A	435	LYS	1
1	A	400	SER	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	53/75 (71%)	36±2 (69±4%)	17±2 (31±4%)	1	15
All	All	2703/3825 (71%)	1860 (69%)	843 (31%)	1	15

All 41 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	401	ILE	51
1	A	380	TYR	50
1	A	438	LEU	47
1	A	436	LYS	43
1	A	445	ARG	43
1	A	412	LEU	41
1	A	443	LYS	41
1	A	375	TYR	39
1	A	373	GLN	38
1	A	399	ASN	35
1	A	426	ARG	34
1	A	437	MET	30
1	A	400	SER	29
1	A	421	LYS	27
1	A	440	PHE	25
1	A	371	LYS	24
1	A	430	ASN	23
1	A	382	SER	22
1	A	439	ASP	19
1	A	435	LYS	19
1	A	433	ARG	15
1	A	369	ASN	15
1	A	385	LEU	15
1	A	384	ARG	14
1	A	383	LEU	13
1	A	420	ILE	13
1	A	418	ARG	12
1	A	372	ARG	11
1	A	405	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	444	GLN	8
1	A	404	CYS	7
1	A	374	LEU	6
1	A	416	VAL	5
1	A	377	LEU	5
1	A	434	ASP	5
1	A	419	ASN	2
1	A	403	GLU	2
1	A	422	ILE	2
1	A	432	LEU	2
1	A	429	GLU	1
1	A	376	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided