



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 08:58 PM UTC

PDB ID : 1FNX / pdb_00001fnx
Title : SOLUTION STRUCTURE OF THE HUC RBD1-RBD2 COMPLEXED
WITH THE AU-RICH ELEMENT
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Deposited on : 2000-08-24

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

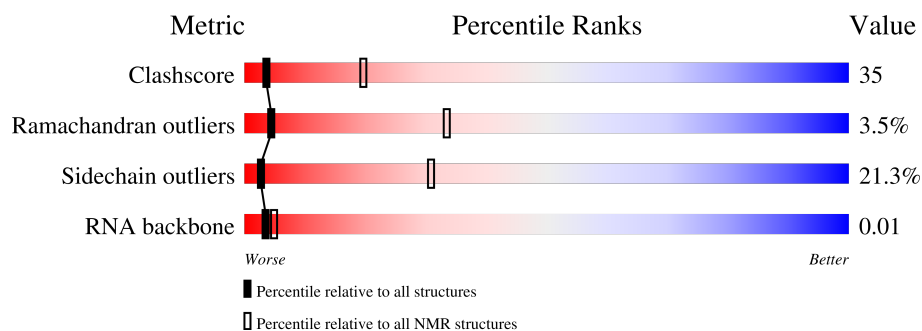
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823
RNA backbone	8273	777

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	R	10	
2	H	174	

2 Ensemble composition and analysis

This entry contains 21 models. Model 21 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	H:38-H:71, H:79-H:119, H:124-H:188, H:198-H:204 (147)	1.66	21

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 6 single-model clusters were found.

Cluster number	Models
1	1, 4, 6, 8, 9, 12, 15, 17, 19, 20, 21
2	3, 5
3	11, 18
Single-model clusters	2; 7; 10; 13; 14; 16

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3022 atoms, of which 1471 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called AU-RICH RNA ELEMENT.

Mol	Chain	Residues	Atoms						Trace
1	R	10	Total	C	H	N	O	P	0
			309	92	104	26	77	10	

- Molecule 2 is a protein called HU ANTIGEN C.

Mol	Chain	Residues	Atoms						Trace
2	H	174	Total	C	H	N	O	S	0
			2713	844	1367	233	264	5	

There is a discrepancy between the modelled and reference sequences:

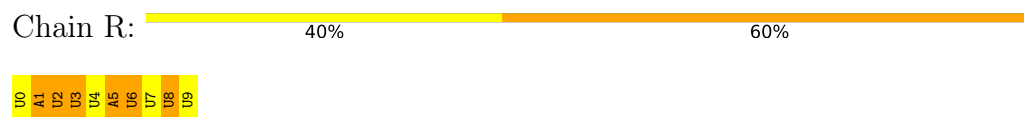
Chain	Residue	Modelled	Actual	Comment	Reference
H	35	MET	ASP	cloning artifact	UNP Q60900

4 Residue-property plots [i](#)

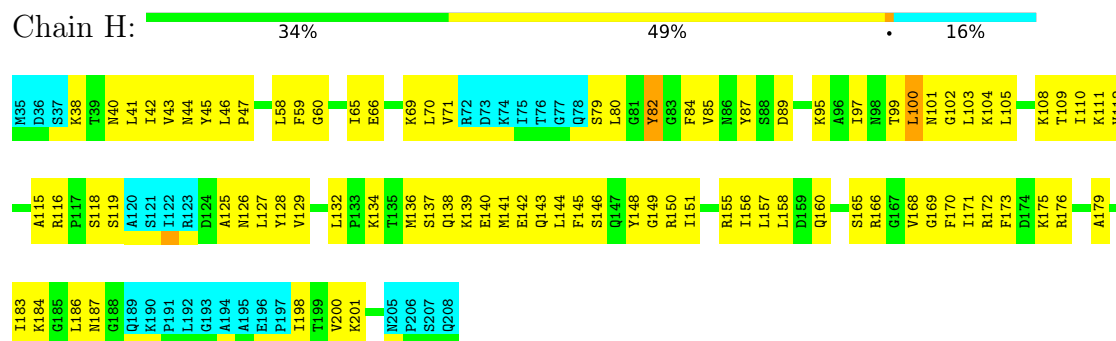
4.1 Average score per residue in the NMR ensemble

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: AU-RICH RNA ELEMENT



• Molecule 2: HU ANTIGEN C

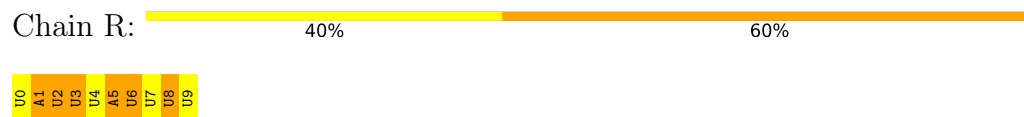


4.2 Scores per residue for each member of the ensemble

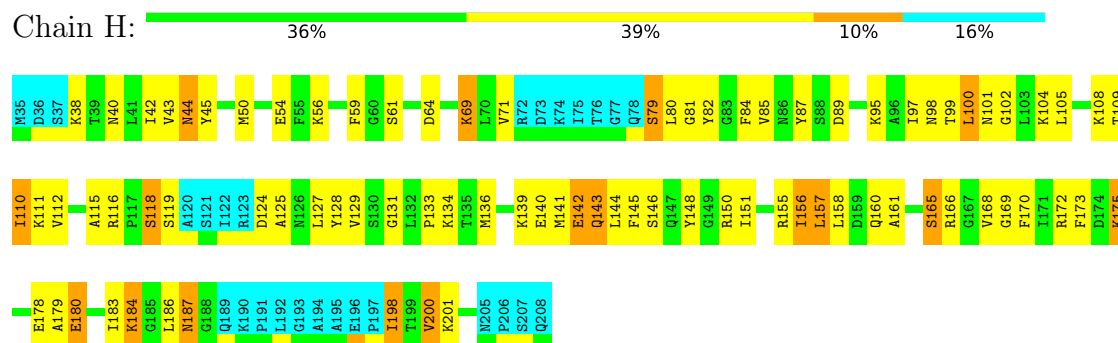
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: AU-RICH RNA ELEMENT

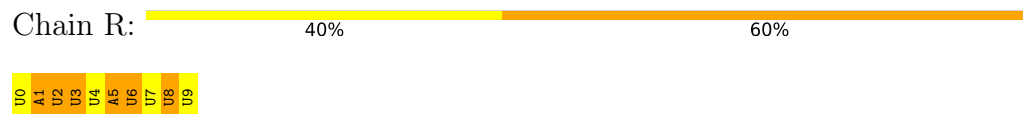


• Molecule 2: HU ANTIGEN C

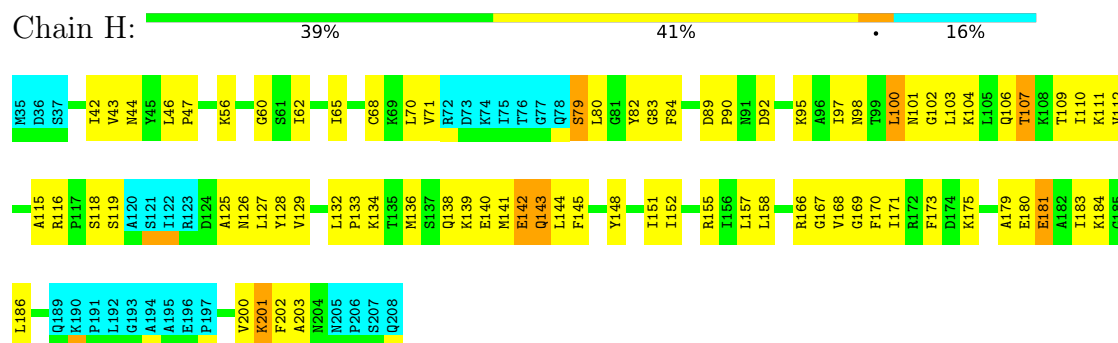


4.2.2 Score per residue for model 2

- Molecule 1: AU-RICH RNA ELEMENT



- Molecule 2: HU ANTIGEN C

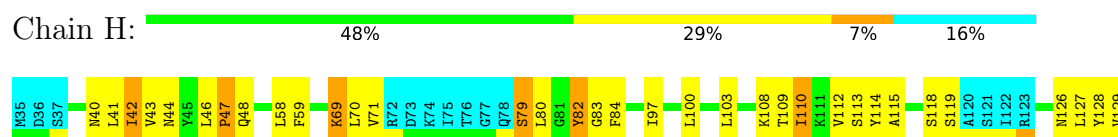


4.2.3 Score per residue for model 3

- Molecule 1: AU-RICH RNA ELEMENT



- Molecule 2: HU ANTIGEN C



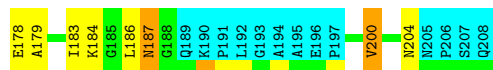


4.2.4 Score per residue for model 4

- Molecule 1: AU-RICH RNA ELEMENT



- Molecule 2: HU ANTIGEN C

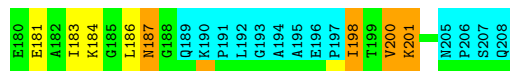
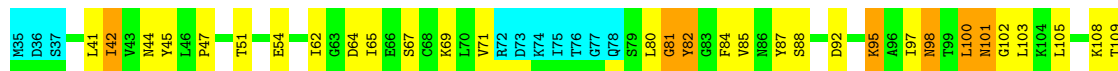


4.2.5 Score per residue for model 5

- Molecule 1: AU-RICH RNA ELEMENT



- Molecule 2: HU ANTIGEN C



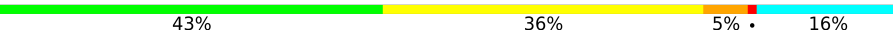
4.2.6 Score per residue for model 6

- Molecule 1: AU-RICH RNA ELEMENT

Chain R: 

U0
A1
U2
U3
U4
A5
U6
U7
U8
U9

- Molecule 2: HU ANTIGEN C

Chain H: 

M35
D36
S37
K38
T39
N40
L41
I42
V43
N44
P47
M50
F59
G60
S61
D64
I65
E66
V71
R72
D73
K74
I75
T76
G77
O78
S79
Y82
G83
F84
V85
S88
K95
A96
I97
N98
T99
L100
N101
G102
L103
K104
T109
I110
K111
V112
S113
Y114
A115
A120

S121
I122
D123
K124
N125
M126
L127
Y128
V129
L132
M136
M141
E142
F145
S146
Q147
Y148
G149
R150
I151
S154
R155
I156
L157
L158
D159
Q160
A161
S165
R166
G167
V168
G169
F170
I171
R172
F173
D174
K175
E178
A179
I183
K184
G185
L186
N187
G188
Q189
K190
P191
L192
G193

A194
A195
E196
P197
T198
T199
V200
N205
P206
S207
Q208

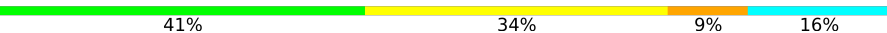
4.2.7 Score per residue for model 7

- Molecule 1: AU-RICH RNA ELEMENT

Chain R: 

U0
A1
U2
U3
U4
A5
U6
U7
U8
U9

- Molecule 2: HU ANTIGEN C

Chain H: 

M35
D36
S37
K38
T39
N40
L41
I42
V43
M44
Y45
L46
P47
Q48
Q52
D53
E54
L58
F59
I65
E66
S67
C68
R69
L70
V71
R72
D73
K74
I75
T76
G77
Q78
S79
L80
G81
Y82
G83
F84
V85
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P90
K95
A96
I97
N98
T99
L100
N101
G102
L103
K104
L105

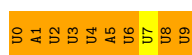
K108
T109
I110
K111
V112
A115
R116
P117
S118
G119
A120
S121
I122
A123
N126
L127
Y128
V129
P133
K134
T135
M136
S137
E140
M141
E142
Q143
L144
F145
S146
Q147
Y148
G149
R150
I151
I156
L157
V168
G169
F170
I171
R172
F173
R176
E180
L183
L186
N187
G188
Q189

K190
P191
L192
G193
A194
A195
E196
P197
V200
K201
N205
P206
S207
Q208

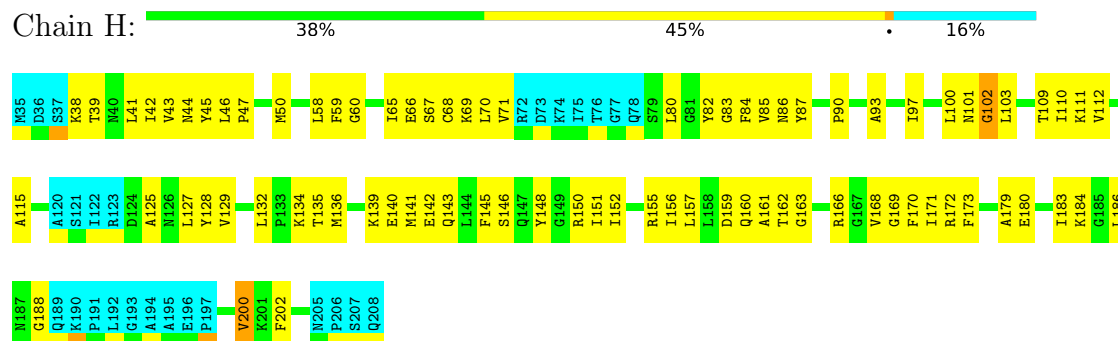
4.2.8 Score per residue for model 8

- Molecule 1: AU-RICH RNA ELEMENT

Chain R: 

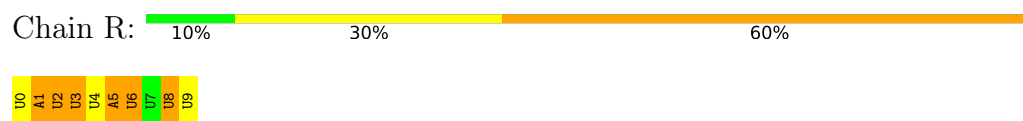


• Molecule 2: HU ANTIGEN C

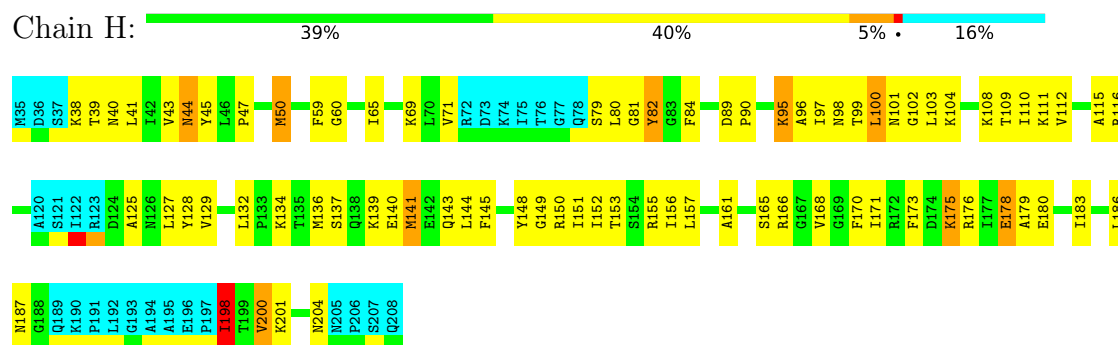


4.2.9 Score per residue for model 9

• Molecule 1: AU-RICH RNA ELEMENT



• Molecule 2: HU ANTIGEN C



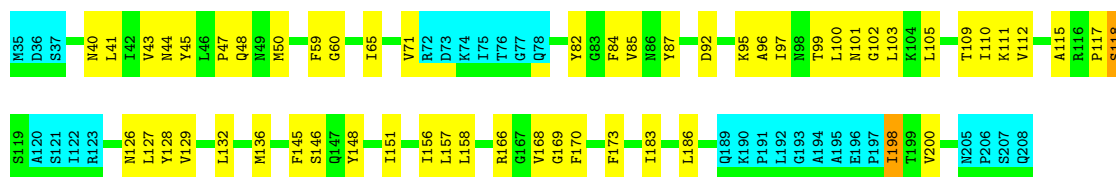
4.2.10 Score per residue for model 10

• Molecule 1: AU-RICH RNA ELEMENT



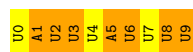
• Molecule 2: HU ANTIGEN C



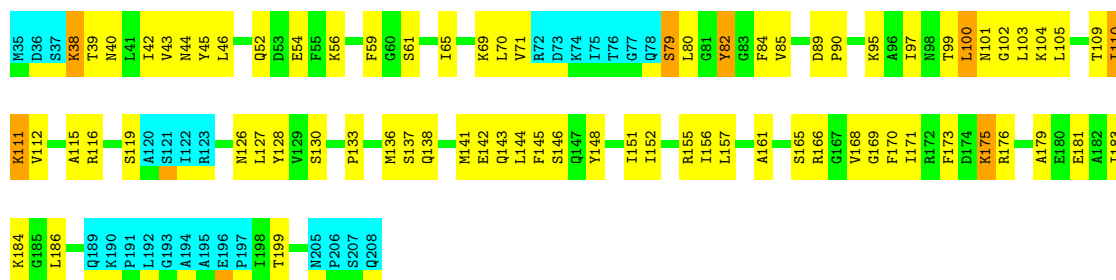


4.2.11 Score per residue for model 11

- Molecule 1: AU-RICH RNA ELEMENT

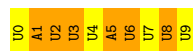


- Molecule 2: HU ANTIGEN C



4.2.12 Score per residue for model 12

- Molecule 1: AU-RICH RNA ELEMENT



- Molecule 2: HU ANTIGEN C



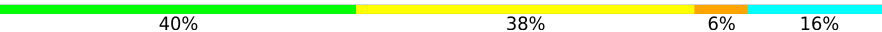
4.2.13 Score per residue for model 13

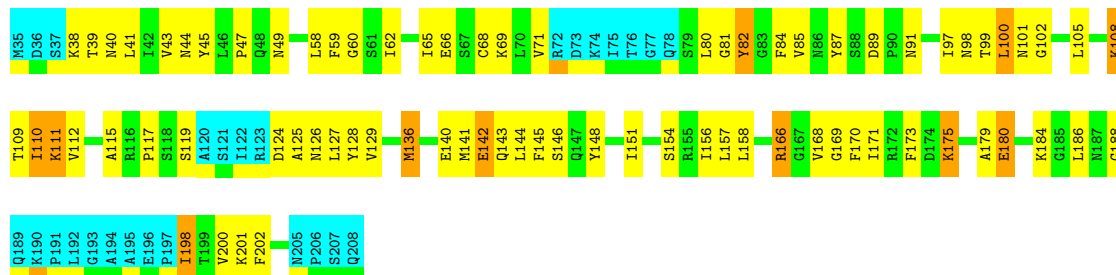
- Molecule 1: AU-RICH RNA ELEMENT

Chain R:  20% 70% 10%



- Molecule 2: HU ANTIGEN C

Chain H:  40% 38% 6% 16%



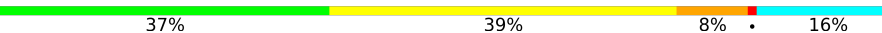
4.2.14 Score per residue for model 14

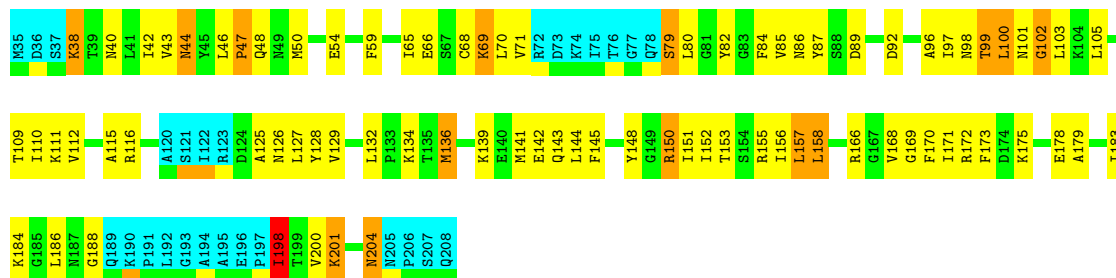
- Molecule 1: AU-RICH RNA ELEMENT

Chain R:  40% 60%



- Molecule 2: HU ANTIGEN C

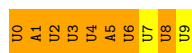
Chain H:  37% 39% 8% 16%



4.2.15 Score per residue for model 15

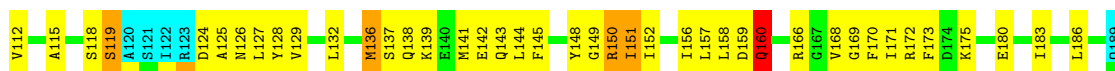
- Molecule 1: AU-RICH RNA ELEMENT

Chain R:  20% 80%



• Molecule 2: HU ANTIGEN C

Chain H: 42% 37% 5% 16%



4.2.16 Score per residue for model 16

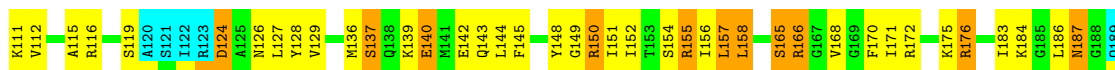
• Molecule 1: AU-RICH RNA ELEMENT

Chain R: 10% 90%



• Molecule 2: HU ANTIGEN C

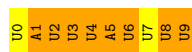
Chain H: 37% 39% 9% 16%



4.2.17 Score per residue for model 17

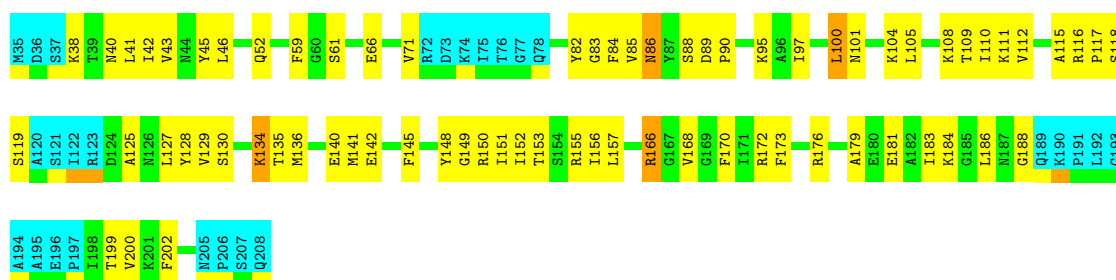
• Molecule 1: AU-RICH RNA ELEMENT

Chain R: 20% 80%



• Molecule 2: HU ANTIGEN C

Chain H: 43% 39% 16%



4.2.18 Score per residue for model 18

- Molecule 1: AU-RICH RNA ELEMENT

Chain R: 20% 80%



- Molecule 2: HU ANTIGEN C

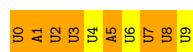
Chain H: 37% 40% 7% 16%



4.2.19 Score per residue for model 19

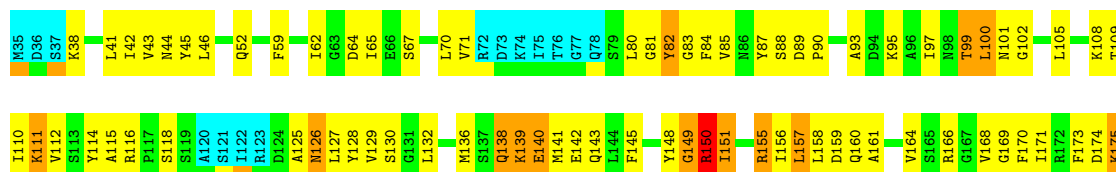
- Molecule 1: AU-RICH RNA ELEMENT

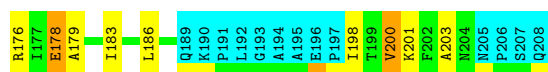
Chain R: 30% 70%



- Molecule 2: HU ANTIGEN C

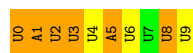
Chain H: 35% 40% 9% 16%



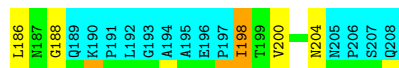


4.2.20 Score per residue for model 20

- Molecule 1: AU-RICH RNA ELEMENT

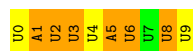


- Molecule 2: HU ANTIGEN C

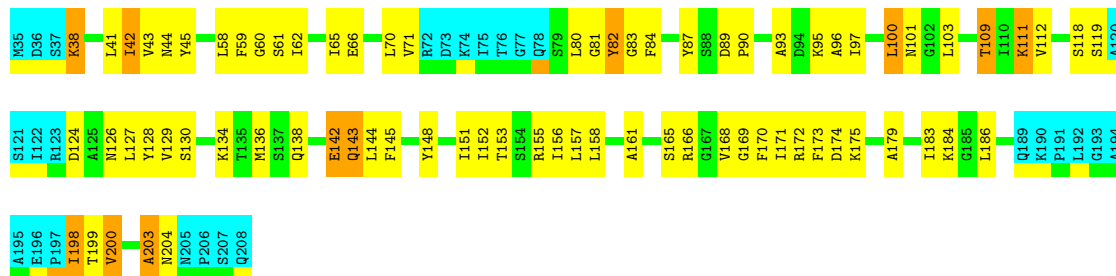


4.2.21 Score per residue for model 21 (medoid)

- Molecule 1: AU-RICH RNA ELEMENT



- Molecule 2: HU ANTIGEN C



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 200 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy. CONFORMER 21 IS THE MINIMIZED AVERAGE STRUCTURE OF CONFORMERS 1-20.*

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

Software name	Classification	Version
CNS	structure solution	0.9
CNS	refinement	0.9

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	R	0.44±0.01	1±0/226 (0.4± 0.0%)	0.72±0.04	0±0/346 (0.0± 0.0%)
2	H	0.43±0.01	0±0/1161 (0.0± 0.0%)	0.68±0.01	0±0/1564 (0.0± 0.0%)
All	All	0.44	21/29127 (0.1%)	0.69	0/40110 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	R	0.0±0.0	0.0±0.2
All	All	0	1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	R	0	U	OP3-P	5.64	1.59	1.48	2	21

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	R	2	U	Sidechain	1

6.2 Too-close contacts [i](#)

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

averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	R	205	104	103	32±7
2	H	1144	1163	1163	89±11
All	All	28329	26607	26586	1934

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:8:U:O4'	2:H:71:VAL:HG22	1.05	1.50	19	13
2:H:157:LEU:HD21	2:H:168:VAL:HB	0.97	1.37	13	10
1:R:2:U:C6	2:H:170:PHE:CZ	0.93	2.57	2	21
1:R:5:A:C2	2:H:80:LEU:HD21	0.89	2.02	5	1
1:R:5:A:N3	2:H:80:LEU:HD21	0.89	1.81	5	2
2:H:40:ASN:ND2	2:H:115:ALA:HB3	0.88	1.82	10	13
2:H:127:LEU:HD22	2:H:183:ILE:HD11	0.88	1.46	4	12
2:H:128:TYR:CE1	2:H:168:VAL:HG11	0.87	2.05	18	20
2:H:136:MET:HB3	2:H:156:ILE:HD13	0.86	1.44	13	14
2:H:105:LEU:HD11	2:H:110:ILE:HD11	0.85	1.45	11	5
1:R:5:A:N3	2:H:80:LEU:HD23	0.85	1.85	9	10
2:H:129:VAL:HG22	2:H:200:VAL:HG23	0.85	1.46	13	20
1:R:5:A:N3	2:H:80:LEU:HD11	0.85	1.87	7	3
2:H:71:VAL:HG21	2:H:82:TYR:CE2	0.83	2.08	6	4
1:R:2:U:O5'	2:H:157:LEU:HD13	0.83	1.72	20	11
1:R:1:A:H4'	2:H:157:LEU:HD21	0.82	1.49	10	4
2:H:145:PHE:HB2	2:H:151:ILE:HD11	0.82	1.49	7	19
2:H:60:GLY:HA2	2:H:65:ILE:HD11	0.82	1.51	6	1
1:R:2:U:C6	2:H:170:PHE:CE1	0.82	2.68	8	2
1:R:2:U:C6	2:H:170:PHE:CE2	0.81	2.68	18	19
2:H:43:VAL:HG22	2:H:112:VAL:HG22	0.81	1.50	1	17
2:H:127:LEU:HD11	2:H:179:ALA:HB1	0.81	1.52	5	14
2:H:157:LEU:HD22	2:H:170:PHE:CE2	0.80	2.12	20	6
1:R:5:A:C4	2:H:80:LEU:HD11	0.80	2.11	7	1
2:H:157:LEU:HD23	2:H:168:VAL:O	0.80	1.76	5	7
2:H:129:VAL:HG12	2:H:132:LEU:HD21	0.80	1.54	9	1
1:R:2:U:C5	2:H:170:PHE:CZ	0.79	2.70	11	21
2:H:127:LEU:HD21	2:H:183:ILE:HD11	0.78	1.55	9	8
2:H:127:LEU:HD21	2:H:179:ALA:HB1	0.78	1.53	4	3
1:R:7:U:C4	2:H:115:ALA:HB1	0.78	2.13	8	3
2:H:80:LEU:HD13	2:H:82:TYR:OH	0.78	1.79	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:7:U:O4	2:H:115:ALA:HB1	0.77	1.79	3	5
2:H:106:GLN:O	2:H:107:THR:HG23	0.77	1.80	2	1
2:H:43:VAL:HG22	2:H:112:VAL:HG13	0.76	1.58	7	6
2:H:141:MET:HE2	2:H:171:ILE:HD11	0.75	1.56	2	2
1:R:1:A:C6	2:H:128:TYR:CE2	0.75	2.75	10	17
1:R:5:A:H4'	1:R:6:U:O5'	0.75	1.80	8	1
2:H:157:LEU:HD11	2:H:168:VAL:HB	0.75	1.57	14	3
1:R:2:U:H5''	1:R:4:U:O3'	0.75	1.82	16	1
2:H:145:PHE:CB	2:H:151:ILE:HD11	0.74	2.12	19	19
1:R:2:U:C5	2:H:170:PHE:CE2	0.74	2.74	8	2
2:H:129:VAL:HG13	2:H:200:VAL:HB	0.74	1.58	13	14
2:H:158:LEU:HD12	2:H:167:GLY:HA2	0.74	1.57	2	3
2:H:68:CYS:SG	2:H:85:VAL:HG22	0.74	2.22	7	1
2:H:71:VAL:HG23	2:H:84:PHE:CZ	0.73	2.18	19	12
2:H:157:LEU:HD21	2:H:170:PHE:CE2	0.73	2.18	7	1
1:R:2:U:C5	2:H:170:PHE:CE1	0.73	2.77	5	18
2:H:80:LEU:HD12	2:H:82:TYR:OH	0.73	1.82	7	2
2:H:59:PHE:CZ	2:H:100:LEU:HD22	0.73	2.19	14	8
2:H:100:LEU:HD12	2:H:103:LEU:HD11	0.73	1.59	12	4
2:H:43:VAL:HG13	2:H:112:VAL:HG22	0.72	1.59	7	5
2:H:80:LEU:HD22	2:H:82:TYR:OH	0.72	1.85	9	3
1:R:8:U:O4'	2:H:71:VAL:HG21	0.72	1.84	4	7
1:R:8:U:C6	2:H:84:PHE:CZ	0.72	2.77	19	17
2:H:125:ALA:HB3	2:H:173:PHE:O	0.71	1.84	1	14
2:H:148:TYR:CE2	2:H:186:LEU:HD21	0.71	2.21	10	3
2:H:59:PHE:CE2	2:H:100:LEU:HD13	0.71	2.20	3	8
2:H:42:ILE:HD11	2:H:82:TYR:CD2	0.71	2.20	18	5
2:H:62:ILE:HD13	2:H:100:LEU:HD11	0.71	1.63	21	2
2:H:71:VAL:HB	2:H:82:TYR:CD1	0.70	2.21	5	2
1:R:1:A:C2	2:H:128:TYR:CD2	0.70	2.79	21	21
2:H:129:VAL:HG22	2:H:200:VAL:CG2	0.70	2.15	16	19
2:H:148:TYR:CZ	2:H:186:LEU:HD21	0.70	2.21	16	12
2:H:186:LEU:O	2:H:198:ILE:HD11	0.69	1.87	3	3
2:H:145:PHE:CE2	2:H:200:VAL:HG21	0.69	2.23	21	3
2:H:157:LEU:HD21	2:H:170:PHE:CZ	0.69	2.22	7	1
1:R:1:A:C5	2:H:128:TYR:CZ	0.69	2.81	10	20
2:H:71:VAL:HB	2:H:82:TYR:CE1	0.69	2.22	13	8
2:H:85:VAL:HG11	2:H:87:TYR:CE2	0.69	2.23	18	4
1:R:4:U:H2'	1:R:4:U:O2	0.69	1.87	5	1
2:H:105:LEU:HD12	2:H:110:ILE:HD12	0.68	1.65	12	1
2:H:157:LEU:CD2	2:H:168:VAL:HB	0.68	2.19	15	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:157:LEU:HD12	2:H:166:ARG:HG3	0.68	1.63	2	2
1:R:8:U:O2'	1:R:9:U:H4'	0.68	1.87	5	1
1:R:2:U:H5'	2:H:157:LEU:HD13	0.68	1.65	13	3
2:H:71:VAL:HG23	2:H:84:PHE:CE2	0.68	2.23	2	5
2:H:127:LEU:CD2	2:H:183:ILE:HD11	0.68	2.19	5	15
1:R:7:U:C5	2:H:115:ALA:HB1	0.68	2.24	8	2
1:R:8:U:C4'	2:H:71:VAL:HG13	0.67	2.19	18	9
1:R:7:U:H2'	1:R:7:U:O2	0.67	1.89	5	1
2:H:145:PHE:CD2	2:H:186:LEU:HD13	0.67	2.25	7	3
1:R:6:U:C5	2:H:152:ILE:HG22	0.67	2.24	11	5
2:H:97:ILE:HG23	2:H:101:ASN:ND2	0.67	2.03	18	4
1:R:3:U:C2	2:H:109:THR:HB	0.67	2.25	20	15
2:H:157:LEU:HD22	2:H:170:PHE:HE2	0.67	1.46	5	3
1:R:1:A:H4'	2:H:157:LEU:HD11	0.66	1.66	2	7
2:H:128:TYR:HE1	2:H:168:VAL:HG11	0.66	1.49	19	13
1:R:8:U:C5	2:H:84:PHE:CE1	0.66	2.83	19	6
2:H:145:PHE:CE2	2:H:186:LEU:HD13	0.66	2.25	8	8
2:H:59:PHE:CE2	2:H:100:LEU:HD22	0.66	2.24	16	3
2:H:71:VAL:HG23	2:H:84:PHE:HZ	0.66	1.50	19	3
1:R:1:A:N1	2:H:204:ASN:HB3	0.65	2.06	21	5
2:H:41:LEU:CD1	2:H:97:ILE:HD11	0.65	2.21	6	2
2:H:136:MET:HE2	2:H:141:MET:HG2	0.65	1.67	7	1
2:H:126:ASN:HD22	2:H:203:ALA:HB2	0.65	1.51	21	1
2:H:85:VAL:HG11	2:H:87:TYR:CZ	0.65	2.27	5	9
1:R:5:A:H2'	2:H:80:LEU:O	0.64	1.92	20	2
2:H:157:LEU:HD22	2:H:157:LEU:O	0.64	1.92	14	2
2:H:42:ILE:CG2	2:H:115:ALA:HB2	0.64	2.23	1	4
2:H:97:ILE:HD12	2:H:114:TYR:CE2	0.64	2.27	3	2
2:H:52:GLN:HG3	2:H:70:LEU:HD13	0.64	1.68	7	1
2:H:128:TYR:CD1	2:H:168:VAL:HG11	0.64	2.28	7	18
2:H:71:VAL:HG23	2:H:84:PHE:HE2	0.64	1.53	2	3
2:H:42:ILE:HD11	2:H:82:TYR:HB2	0.63	1.69	5	1
2:H:40:ASN:HD22	2:H:115:ALA:HB3	0.63	1.53	14	7
1:R:8:U:C4	2:H:84:PHE:CE2	0.63	2.86	5	11
1:R:8:U:C4'	2:H:71:VAL:HG21	0.62	2.24	7	3
1:R:8:U:C6	2:H:84:PHE:CE1	0.62	2.87	3	4
2:H:157:LEU:HG	2:H:166:ARG:HB2	0.62	1.70	8	11
2:H:157:LEU:HD12	2:H:168:VAL:O	0.62	1.94	7	1
2:H:158:LEU:C	2:H:158:LEU:HD22	0.62	2.20	14	1
2:H:42:ILE:HD11	2:H:82:TYR:HD2	0.62	1.53	18	3
2:H:145:PHE:HB2	2:H:151:ILE:CD1	0.62	2.25	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:109:THR:O	2:H:109:THR:HG22	0.61	1.94	7	4
2:H:157:LEU:CD1	2:H:168:VAL:HB	0.61	2.24	14	3
1:R:8:U:H5'	2:H:82:TYR:OH	0.61	1.96	3	1
1:R:8:U:H1'	1:R:9:U:O5'	0.61	1.96	8	1
2:H:157:LEU:HD22	2:H:170:PHE:CZ	0.61	2.30	13	3
2:H:82:TYR:CD1	2:H:82:TYR:N	0.61	2.69	5	6
1:R:1:A:C2	2:H:128:TYR:CG	0.60	2.89	21	17
2:H:71:VAL:HG23	2:H:84:PHE:HE1	0.60	1.55	4	1
2:H:59:PHE:CB	2:H:65:ILE:HD11	0.60	2.26	7	1
1:R:2:U:H5'	2:H:157:LEU:CD2	0.60	2.27	7	1
1:R:3:U:C2	2:H:45:TYR:CD2	0.60	2.89	1	8
1:R:1:A:C4'	2:H:157:LEU:HD11	0.60	2.27	2	4
2:H:71:VAL:HG23	2:H:84:PHE:CE1	0.60	2.31	13	11
2:H:151:ILE:HG21	2:H:171:ILE:CG2	0.60	2.26	19	1
1:R:1:A:C4	2:H:128:TYR:CE1	0.60	2.90	7	15
1:R:9:U:OP1	2:H:71:VAL:CG2	0.59	2.50	3	2
2:H:65:ILE:HG23	2:H:85:VAL:HG13	0.59	1.74	15	5
2:H:46:LEU:HD12	2:H:70:LEU:HG	0.59	1.73	8	3
2:H:129:VAL:CG2	2:H:200:VAL:HG23	0.59	2.26	2	2
2:H:157:LEU:HD12	2:H:170:PHE:CE2	0.59	2.31	14	3
2:H:41:LEU:HD11	2:H:97:ILE:HD11	0.59	1.74	16	1
2:H:129:VAL:CG1	2:H:132:LEU:HD21	0.59	2.25	9	1
2:H:97:ILE:HD13	2:H:112:VAL:HB	0.59	1.74	2	1
1:R:2:U:O5'	2:H:157:LEU:CD1	0.59	2.50	21	8
2:H:103:LEU:HB2	2:H:110:ILE:HG22	0.59	1.73	14	1
2:H:105:LEU:CD1	2:H:110:ILE:HD11	0.59	2.27	15	5
1:R:5:A:C4	2:H:80:LEU:HD21	0.59	2.33	14	2
2:H:105:LEU:CD1	2:H:110:ILE:HD13	0.59	2.28	17	1
2:H:154:SER:HB2	2:H:171:ILE:HD13	0.59	1.74	18	4
2:H:80:LEU:HB3	2:H:82:TYR:CZ	0.58	2.33	2	3
2:H:146:SER:N	2:H:151:ILE:HD11	0.58	2.13	3	6
2:H:59:PHE:HB2	2:H:65:ILE:HD11	0.58	1.74	7	1
2:H:156:ILE:HG23	2:H:168:VAL:O	0.58	1.97	14	15
2:H:157:LEU:HD11	2:H:166:ARG:HG3	0.58	1.74	4	2
1:R:1:A:N3	2:H:128:TYR:CG	0.58	2.72	5	15
1:R:5:A:N3	2:H:80:LEU:CD2	0.58	2.67	19	3
2:H:103:LEU:HB2	2:H:110:ILE:CG2	0.58	2.28	8	4
1:R:5:A:C4	2:H:80:LEU:HD23	0.58	2.34	19	2
2:H:97:ILE:HD12	2:H:114:TYR:CZ	0.58	2.34	4	1
2:H:188:GLY:HA3	2:H:198:ILE:HG13	0.58	1.76	13	3
1:R:8:U:C1'	2:H:71:VAL:HG22	0.57	2.29	12	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:105:LEU:HD11	2:H:110:ILE:CG1	0.57	2.30	10	1
1:R:1:A:O5'	2:H:157:LEU:HD21	0.57	1.99	16	1
2:H:50:MET:HE3	2:H:55:PHE:HA	0.57	1.75	4	2
2:H:175:LYS:CE	2:H:178:GLU:HB2	0.57	2.29	4	1
1:R:6:U:O4'	2:H:44:ASN:HB3	0.57	2.00	8	4
2:H:128:TYR:CE1	2:H:168:VAL:CG1	0.57	2.88	3	13
2:H:41:LEU:HG	2:H:97:ILE:HD11	0.57	1.75	3	1
2:H:65:ILE:HG21	2:H:68:CYS:SG	0.57	2.40	7	4
2:H:94:ASP:HA	2:H:97:ILE:HD12	0.57	1.77	15	2
2:H:43:VAL:CG1	2:H:112:VAL:HG22	0.56	2.30	7	1
2:H:119:SER:O	2:H:175:LYS:NZ	0.56	2.35	13	2
2:H:65:ILE:CG2	2:H:68:CYS:SG	0.56	2.93	7	2
1:R:8:U:C5	2:H:84:PHE:CE2	0.56	2.94	4	1
2:H:96:ALA:O	2:H:100:LEU:HD12	0.56	2.00	16	3
2:H:87:TYR:CD2	2:H:93:ALA:HA	0.56	2.35	8	2
2:H:148:TYR:CE1	2:H:186:LEU:HD21	0.56	2.35	8	7
1:R:3:U:C2	2:H:45:TYR:CG	0.56	2.94	20	5
2:H:151:ILE:HG21	2:H:154:SER:HB3	0.56	1.76	16	1
2:H:71:VAL:HG11	2:H:82:TYR:OH	0.56	2.01	4	2
1:R:2:U:H5'	2:H:157:LEU:CD1	0.56	2.31	2	3
2:H:43:VAL:CG2	2:H:112:VAL:HG22	0.55	2.29	13	3
2:H:138:GLN:CB	2:H:155:ARG:HA	0.55	2.30	19	1
1:R:5:A:O2'	1:R:6:U:P	0.55	2.65	17	5
2:H:141:MET:CE	2:H:171:ILE:HD11	0.55	2.30	2	1
2:H:103:LEU:HB3	2:H:110:ILE:HD12	0.55	1.77	5	1
2:H:151:ILE:CG2	2:H:171:ILE:HG22	0.55	2.31	19	2
2:H:92:ASP:HA	2:H:95:LYS:HG2	0.55	1.77	10	1
2:H:97:ILE:HG23	2:H:101:ASN:HD22	0.55	1.61	2	2
2:H:157:LEU:O	2:H:157:LEU:HG	0.55	2.02	19	7
1:R:1:A:C4'	2:H:157:LEU:HD21	0.55	2.31	16	3
1:R:0:U:O2'	1:R:1:A:P	0.55	2.64	5	2
1:R:6:U:C5	2:H:152:ILE:CG2	0.55	2.89	8	3
2:H:47:PRO:HB2	2:H:50:MET:HB2	0.55	1.76	14	1
2:H:100:LEU:HB2	2:H:112:VAL:HG21	0.55	1.78	3	1
2:H:44:ASN:CG	2:H:82:TYR:HB3	0.55	2.27	10	2
1:R:2:U:H4'	2:H:157:LEU:HB2	0.55	1.79	8	5
1:R:8:U:C4	2:H:84:PHE:CE1	0.54	2.95	15	3
1:R:5:A:N3	2:H:80:LEU:HA	0.54	2.17	18	1
2:H:157:LEU:HG	2:H:157:LEU:O	0.54	2.02	17	7
1:R:1:A:H5'	2:H:168:VAL:HG21	0.54	1.78	20	4
2:H:129:VAL:HG22	2:H:200:VAL:CB	0.54	2.31	21	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:1:A:C5'	2:H:157:LEU:HD11	0.54	2.32	2	4
1:R:6:U:C5	2:H:153:THR:HG23	0.54	2.38	4	1
2:H:71:VAL:CG2	2:H:84:PHE:CZ	0.54	2.91	17	11
2:H:97:ILE:O	2:H:101:ASN:HB2	0.54	2.03	9	14
2:H:71:VAL:CG1	2:H:82:TYR:CE1	0.54	2.90	5	1
1:R:2:U:O2'	1:R:3:U:H5'	0.54	2.03	6	3
2:H:157:LEU:HD12	2:H:157:LEU:H	0.54	1.63	7	1
2:H:80:LEU:HB3	2:H:82:TYR:CE2	0.54	2.38	11	1
1:R:1:A:C5	2:H:128:TYR:CE2	0.54	2.96	10	15
2:H:134:LYS:HG3	2:H:158:LEU:HD11	0.54	1.78	20	2
2:H:142:GLU:HG2	2:H:143:GLN:N	0.54	2.16	2	3
2:H:47:PRO:HD3	2:H:110:ILE:HD11	0.54	1.80	20	2
1:R:7:U:O2	1:R:7:U:C2'	0.54	2.56	5	1
2:H:100:LEU:HD23	2:H:103:LEU:CD1	0.54	2.33	6	1
2:H:80:LEU:HB3	2:H:82:TYR:CE1	0.54	2.37	8	1
2:H:47:PRO:HB2	2:H:50:MET:CB	0.54	2.33	14	1
2:H:97:ILE:HG23	2:H:101:ASN:CG	0.53	2.28	5	2
2:H:152:ILE:O	2:H:153:THR:HG23	0.53	2.02	9	2
2:H:117:PRO:O	2:H:118:SER:CB	0.53	2.55	10	1
2:H:103:LEU:HB2	2:H:110:ILE:HB	0.53	1.80	2	4
2:H:132:LEU:HB3	2:H:136:MET:SD	0.53	2.44	6	5
2:H:126:ASN:O	2:H:127:LEU:HD23	0.53	2.03	4	2
2:H:100:LEU:HD23	2:H:103:LEU:HD11	0.53	1.79	6	4
2:H:136:MET:CB	2:H:156:ILE:HD13	0.53	2.30	5	4
2:H:187:ASN:HA	2:H:200:VAL:HG12	0.53	1.81	6	1
2:H:42:ILE:HG21	2:H:115:ALA:HB2	0.53	1.80	11	1
2:H:157:LEU:CD2	2:H:170:PHE:CZ	0.53	2.92	11	1
1:R:1:A:H4'	2:H:157:LEU:CD1	0.53	2.33	20	9
1:R:2:U:H4'	2:H:157:LEU:CB	0.53	2.33	3	5
2:H:128:TYR:HA	2:H:170:PHE:CD2	0.53	2.38	8	1
1:R:4:U:H6	1:R:4:U:O5'	0.53	1.85	17	2
2:H:145:PHE:CZ	2:H:200:VAL:HG21	0.53	2.39	21	1
1:R:8:U:C2	2:H:84:PHE:CE2	0.53	2.97	10	2
1:R:6:U:O2	2:H:42:ILE:HG23	0.53	2.04	21	2
2:H:59:PHE:CE1	2:H:100:LEU:HD22	0.53	2.39	14	1
1:R:8:U:H4'	2:H:71:VAL:HG13	0.52	1.80	12	6
2:H:59:PHE:CD2	2:H:85:VAL:HG21	0.52	2.39	6	2
2:H:136:MET:HE2	2:H:141:MET:SD	0.52	2.44	9	3
1:R:1:A:O5'	2:H:166:ARG:HG2	0.52	2.04	17	3
2:H:145:PHE:HB3	2:H:173:PHE:CZ	0.52	2.39	10	15
1:R:7:U:O2	2:H:116:ARG:HD3	0.52	2.03	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:125:ALA:HB1	2:H:173:PHE:HB2	0.52	1.82	9	1
1:R:1:A:O3'	1:R:2:U:C6	0.52	2.63	3	1
2:H:42:ILE:HB	2:H:84:PHE:CD2	0.52	2.40	21	2
1:R:1:A:C4	2:H:128:TYR:CD1	0.52	2.97	7	13
1:R:1:A:N1	2:H:204:ASN:HB2	0.52	2.19	14	1
1:R:1:A:C5'	2:H:157:LEU:HD21	0.52	2.35	16	1
1:R:6:U:OP2	2:H:45:TYR:CE2	0.52	2.62	11	1
2:H:44:ASN:OD1	2:H:82:TYR:CD2	0.52	2.63	19	1
2:H:198:ILE:HG13	2:H:198:ILE:O	0.52	2.05	13	3
1:R:8:U:C6	2:H:71:VAL:HG22	0.52	2.40	20	8
2:H:60:GLY:CA	2:H:65:ILE:HD11	0.52	2.32	6	1
2:H:126:ASN:ND2	2:H:203:ALA:HB2	0.52	2.19	21	3
2:H:118:SER:OG	2:H:119:SER:N	0.51	2.43	2	3
2:H:145:PHE:CB	2:H:171:ILE:HG21	0.51	2.35	21	2
2:H:70:LEU:HD23	2:H:70:LEU:C	0.51	2.30	11	5
2:H:102:GLY:HA2	2:H:111:LYS:HD2	0.51	1.80	7	1
2:H:141:MET:HE2	2:H:156:ILE:HG13	0.51	1.83	1	1
2:H:71:VAL:CB	2:H:82:TYR:CE1	0.51	2.93	13	2
1:R:1:A:N9	2:H:128:TYR:CE1	0.51	2.79	7	3
2:H:129:VAL:HB	2:H:141:MET:HE1	0.51	1.82	6	1
2:H:87:TYR:CD1	2:H:92:ASP:HB3	0.51	2.40	12	2
2:H:105:LEU:HD12	2:H:110:ILE:HD13	0.51	1.82	17	2
1:R:8:U:C5	2:H:84:PHE:CZ	0.51	2.99	19	3
2:H:101:ASN:O	2:H:111:LYS:NZ	0.51	2.43	2	10
2:H:46:LEU:HD11	2:H:83:GLY:CA	0.51	2.36	8	3
2:H:128:TYR:HA	2:H:170:PHE:CD1	0.51	2.41	21	5
2:H:43:VAL:HG11	2:H:110:ILE:HD11	0.51	1.83	16	1
1:R:3:U:O2	2:H:109:THR:HB	0.51	2.05	14	6
2:H:96:ALA:C	2:H:100:LEU:HD12	0.51	2.31	21	2
2:H:60:GLY:HA2	2:H:65:ILE:CD1	0.51	2.36	9	8
2:H:142:GLU:HA	2:H:151:ILE:CD1	0.51	2.36	7	1
2:H:152:ILE:HB	2:H:172:ARG:HG3	0.51	1.83	14	1
1:R:8:U:OP1	2:H:71:VAL:HG11	0.51	2.06	15	1
2:H:41:LEU:HD13	2:H:114:TYR:HA	0.50	1.81	19	2
2:H:41:LEU:O	2:H:84:PHE:HA	0.50	2.06	20	8
2:H:80:LEU:HB2	2:H:82:TYR:CE1	0.50	2.41	18	1
2:H:103:LEU:HB2	2:H:110:ILE:HG23	0.50	1.83	18	1
2:H:60:GLY:HA2	2:H:65:ILE:HD13	0.50	1.83	10	1
2:H:153:THR:OG1	2:H:172:ARG:NH1	0.50	2.36	12	1
2:H:126:ASN:HB2	2:H:172:ARG:NH1	0.50	2.21	15	1
2:H:70:LEU:HA	2:H:83:GLY:HA2	0.50	1.83	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:183:ILE:HD13	2:H:201:LYS:HA	0.50	1.82	1	3
2:H:198:ILE:O	2:H:198:ILE:HG13	0.50	2.06	9	5
2:H:157:LEU:HD22	2:H:157:LEU:C	0.50	2.32	16	1
1:R:0:U:O3'	1:R:1:A:H3'	0.50	2.07	18	1
2:H:153:THR:OG1	2:H:172:ARG:NE	0.50	2.39	21	1
2:H:168:VAL:CG1	2:H:169:GLY:N	0.50	2.74	7	2
1:R:7:U:H1'	1:R:8:U:OP1	0.50	2.06	3	1
1:R:8:U:C2	2:H:84:PHE:CE1	0.50	3.00	6	3
2:H:104:LYS:HA	2:H:109:THR:HA	0.50	1.84	20	3
2:H:105:LEU:HB2	2:H:108:LYS:O	0.50	2.07	18	3
2:H:116:ARG:HB3	2:H:117:PRO:HD2	0.49	1.83	20	3
2:H:89:ASP:CG	2:H:90:PRO:HD2	0.49	2.32	7	9
2:H:50:MET:HE2	2:H:54:GLU:HB3	0.49	1.83	16	1
2:H:157:LEU:CD1	2:H:166:ARG:HG2	0.49	2.37	20	1
2:H:137:SER:HB3	2:H:140:GLU:HG2	0.49	1.83	5	1
2:H:99:THR:HG22	2:H:100:LEU:HG	0.49	1.85	14	1
1:R:6:U:O2'	1:R:7:U:P	0.49	2.70	12	4
1:R:8:U:O4'	2:H:71:VAL:CG2	0.49	2.56	9	7
1:R:3:U:O2'	2:H:45:TYR:OH	0.49	2.30	7	1
2:H:157:LEU:HD11	2:H:166:ARG:HD2	0.49	1.83	8	1
2:H:133:PRO:HD2	2:H:136:MET:SD	0.49	2.48	7	5
2:H:151:ILE:HG12	2:H:173:PHE:CE1	0.49	2.42	12	5
2:H:100:LEU:CB	2:H:112:VAL:HG21	0.49	2.37	3	1
1:R:3:U:C2	2:H:45:TYR:CD1	0.49	3.01	10	1
2:H:116:ARG:CB	2:H:117:PRO:HD2	0.49	2.37	18	1
1:R:8:U:H5	2:H:42:ILE:HD12	0.49	1.67	3	1
1:R:8:U:O4'	2:H:71:VAL:HA	0.49	2.07	5	1
2:H:134:LYS:HE2	2:H:135:THR:HG23	0.49	1.84	17	1
2:H:145:PHE:CD2	2:H:171:ILE:HG13	0.49	2.42	6	2
2:H:85:VAL:CG1	2:H:87:TYR:CZ	0.49	2.96	5	3
2:H:157:LEU:HD12	2:H:166:ARG:CG	0.49	2.38	11	2
1:R:7:U:C2'	1:R:7:U:O2	0.49	2.61	14	1
2:H:105:LEU:HD11	2:H:110:ILE:CD1	0.49	2.34	4	1
2:H:170:PHE:O	2:H:171:ILE:HD13	0.49	2.07	14	3
2:H:59:PHE:O	2:H:65:ILE:HD11	0.49	2.07	21	2
2:H:136:MET:HG3	2:H:156:ILE:CD1	0.49	2.38	21	6
2:H:157:LEU:HD21	2:H:168:VAL:CB	0.49	2.31	5	1
1:R:6:U:O2'	1:R:7:U:H6	0.49	1.91	10	1
2:H:154:SER:O	2:H:155:ARG:HB3	0.49	2.08	16	1
2:H:188:GLY:HA3	2:H:198:ILE:O	0.49	2.07	14	1
2:H:128:TYR:CD1	2:H:168:VAL:CG1	0.48	2.96	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:175:LYS:HE2	2:H:178:GLU:CD	0.48	2.33	4	1
1:R:2:U:H4'	2:H:157:LEU:HB3	0.48	1.84	5	1
2:H:39:THR:O	2:H:86:ASN:HA	0.48	2.08	8	1
2:H:157:LEU:CD2	2:H:170:PHE:CE2	0.48	2.96	11	1
1:R:8:U:H4'	2:H:71:VAL:HG21	0.48	1.84	3	2
2:H:47:PRO:HG2	2:H:50:MET:CB	0.48	2.38	10	4
2:H:152:ILE:HD11	2:H:174:ASP:OD1	0.48	2.08	21	1
2:H:71:VAL:CG2	2:H:84:PHE:HZ	0.48	2.21	17	8
1:R:7:U:C2	2:H:116:ARG:HD3	0.48	2.42	5	1
2:H:124:ASP:HB2	2:H:176:ARG:CG	0.48	2.38	16	1
1:R:1:A:O3'	1:R:2:U:H6	0.48	1.91	12	6
1:R:8:U:H1'	1:R:9:U:OP1	0.48	2.08	3	2
2:H:157:LEU:HG	2:H:166:ARG:CB	0.48	2.39	8	2
2:H:137:SER:HB3	2:H:140:GLU:CG	0.48	2.38	5	1
2:H:69:LYS:HB3	2:H:84:PHE:CD1	0.48	2.44	1	3
2:H:149:GLY:O	2:H:150:ARG:C	0.48	2.56	20	3
2:H:44:ASN:OD1	2:H:45:TYR:CD2	0.48	2.66	7	1
2:H:41:LEU:CG	2:H:97:ILE:HD11	0.48	2.39	3	1
2:H:129:VAL:HG22	2:H:200:VAL:HB	0.48	1.86	21	1
2:H:138:GLN:OE1	2:H:155:ARG:NH1	0.48	2.44	3	2
2:H:126:ASN:C	2:H:127:LEU:HD23	0.48	2.34	16	2
2:H:97:ILE:HG12	2:H:112:VAL:HG11	0.48	1.85	8	1
2:H:157:LEU:CD1	2:H:170:PHE:CE2	0.48	2.97	10	2
2:H:156:ILE:HA	2:H:169:GLY:HA2	0.48	1.85	11	6
2:H:71:VAL:CG2	2:H:82:TYR:CE2	0.48	2.93	17	2
1:R:5:A:H4'	1:R:6:U:OP1	0.47	2.09	3	3
1:R:4:U:O2'	1:R:5:A:P	0.47	2.72	8	1
2:H:180:GLU:HG3	2:H:202:PHE:CE2	0.47	2.43	13	1
2:H:43:VAL:HG12	2:H:110:ILE:HG12	0.47	1.86	14	1
2:H:115:ALA:O	2:H:116:ARG:HD2	0.47	2.09	14	1
2:H:157:LEU:HD12	2:H:166:ARG:HD3	0.47	1.85	19	1
2:H:136:MET:SD	2:H:141:MET:HG3	0.47	2.49	20	1
2:H:141:MET:SD	2:H:156:ILE:HD11	0.47	2.48	20	1
2:H:145:PHE:HE2	2:H:200:VAL:HG21	0.47	1.69	21	1
1:R:8:U:O2'	1:R:9:U:H5''	0.47	2.10	3	1
2:H:96:ALA:HB1	2:H:100:LEU:HD12	0.47	1.86	14	1
1:R:2:U:N1	2:H:170:PHE:CE2	0.47	2.82	18	10
2:H:97:ILE:O	2:H:101:ASN:N	0.47	2.47	6	3
2:H:136:MET:CG	2:H:156:ILE:HD13	0.47	2.40	8	1
1:R:1:A:H5''	2:H:157:LEU:HD11	0.47	1.87	11	2
2:H:157:LEU:HD12	2:H:166:ARG:HG2	0.47	1.86	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:97:ILE:O	2:H:101:ASN:CB	0.47	2.63	14	1
2:H:137:SER:CB	2:H:140:GLU:CD	0.47	2.88	7	1
2:H:96:ALA:O	2:H:100:LEU:HD22	0.47	2.09	9	1
1:R:6:U:H4'	1:R:7:U:OP1	0.47	2.10	10	1
2:H:101:ASN:C	2:H:111:LYS:HG2	0.47	2.35	18	1
1:R:6:U:O2'	2:H:42:ILE:HD11	0.47	2.09	2	1
2:H:142:GLU:O	2:H:146:SER:N	0.47	2.45	6	1
2:H:137:SER:HB3	2:H:140:GLU:CD	0.47	2.35	7	1
2:H:100:LEU:HB2	2:H:112:VAL:CG2	0.47	2.40	8	1
2:H:105:LEU:HD11	2:H:110:ILE:HG12	0.47	1.86	10	1
2:H:176:ARG:HG2	2:H:177:ILE:N	0.47	2.25	12	1
2:H:129:VAL:O	2:H:168:VAL:HG13	0.47	2.10	20	2
1:R:4:U:O2	1:R:4:U:C2'	0.47	2.57	5	1
1:R:7:U:OP1	2:H:82:TYR:CE2	0.47	2.68	13	1
2:H:96:ALA:HB1	2:H:100:LEU:CD1	0.47	2.40	14	1
2:H:165:SER:O	2:H:166:ARG:HD3	0.47	2.10	20	1
2:H:159:ASP:OD1	2:H:160:GLN:N	0.47	2.45	3	2
2:H:145:PHE:C	2:H:151:ILE:HD11	0.47	2.35	20	2
1:R:8:U:C2	2:H:84:PHE:CZ	0.47	3.02	6	4
2:H:142:GLU:HB2	2:H:154:SER:OG	0.47	2.10	6	2
1:R:5:A:N6	2:H:79:SER:O	0.47	2.48	12	1
2:H:139:LYS:NZ	2:H:140:GLU:OE2	0.47	2.46	19	1
2:H:82:TYR:HB2	2:H:84:PHE:CZ	0.46	2.45	7	1
1:R:7:U:C6	1:R:8:U:C5	0.46	3.03	19	1
2:H:46:LEU:HG	2:H:83:GLY:N	0.46	2.25	2	1
2:H:43:VAL:O	2:H:82:TYR:HA	0.46	2.09	3	2
1:R:4:U:O2	2:H:172:ARG:HB2	0.46	2.11	5	1
1:R:8:U:N1	2:H:84:PHE:CE2	0.46	2.84	8	1
2:H:183:ILE:HG23	2:H:200:VAL:O	0.46	2.11	17	2
1:R:1:A:H5''	2:H:166:ARG:HD3	0.46	1.86	5	1
1:R:2:U:C6	1:R:2:U:OP2	0.46	2.69	8	3
2:H:175:LYS:NZ	2:H:178:GLU:OE1	0.46	2.45	9	2
1:R:1:A:C5'	2:H:166:ARG:HG2	0.46	2.40	16	1
2:H:43:VAL:CG1	2:H:110:ILE:HG23	0.46	2.41	17	1
1:R:2:U:C5'	2:H:157:LEU:HD13	0.46	2.40	2	2
2:H:44:ASN:O	2:H:45:TYR:HB2	0.46	2.10	7	2
2:H:83:GLY:C	2:H:84:PHE:CD1	0.46	2.93	8	1
2:H:145:PHE:CE1	2:H:186:LEU:HD13	0.46	2.45	14	1
2:H:46:LEU:CD1	2:H:70:LEU:HG	0.46	2.40	4	1
2:H:38:LYS:O	2:H:39:THR:HG23	0.46	2.10	6	1
2:H:70:LEU:HD23	2:H:71:VAL:O	0.46	2.11	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:95:LYS:O	2:H:98:ASN:HB2	0.46	2.11	5	2
2:H:129:VAL:CB	2:H:141:MET:HE1	0.46	2.40	6	1
2:H:39:THR:O	2:H:41:LEU:HD22	0.46	2.11	7	1
1:R:2:U:H5'	2:H:157:LEU:HD12	0.46	1.88	1	2
2:H:187:ASN:HB3	2:H:200:VAL:O	0.46	2.11	4	3
2:H:41:LEU:HD22	2:H:41:LEU:N	0.46	2.25	3	3
2:H:137:SER:HB3	2:H:140:GLU:HB2	0.46	1.87	16	1
2:H:97:ILE:HG13	2:H:114:TYR:CE2	0.46	2.44	19	1
2:H:126:ASN:HB2	2:H:172:ARG:CD	0.46	2.41	3	1
2:H:42:ILE:HD11	2:H:82:TYR:CB	0.46	2.41	5	1
2:H:136:MET:HG3	2:H:156:ILE:HD13	0.46	1.87	21	2
1:R:6:U:O4'	2:H:44:ASN:HB2	0.46	2.11	3	1
1:R:2:U:P	2:H:157:LEU:HD13	0.46	2.50	20	2
2:H:69:LYS:HG3	2:H:70:LEU:N	0.46	2.26	8	2
2:H:176:ARG:HD2	2:H:202:PHE:CE2	0.46	2.46	18	1
2:H:47:PRO:O	2:H:49:ASN:N	0.46	2.45	4	1
2:H:62:ILE:HD11	2:H:100:LEU:HD21	0.45	1.88	13	4
2:H:175:LYS:HE3	2:H:178:GLU:HB2	0.45	1.88	4	1
2:H:127:LEU:O	2:H:170:PHE:HA	0.45	2.11	13	2
1:R:9:U:H5'	2:H:69:LYS:HG2	0.45	1.87	8	1
2:H:82:TYR:N	2:H:82:TYR:HD1	0.45	2.08	8	1
2:H:151:ILE:HG21	2:H:171:ILE:HG22	0.45	1.86	19	1
2:H:43:VAL:N	2:H:83:GLY:O	0.45	2.49	8	3
2:H:46:LEU:CD2	2:H:110:ILE:HD11	0.45	2.41	8	1
2:H:109:THR:O	2:H:109:THR:CG2	0.45	2.64	7	1
1:R:1:A:O5'	2:H:166:ARG:HD2	0.45	2.12	8	1
2:H:40:ASN:HD21	2:H:115:ALA:HB3	0.45	1.62	10	1
2:H:157:LEU:CD1	2:H:170:PHE:CZ	0.45	2.99	14	1
1:R:7:U:O4	2:H:115:ALA:CB	0.45	2.61	5	1
2:H:157:LEU:HD13	2:H:168:VAL:HB	0.45	1.87	7	1
2:H:172:ARG:NE	2:H:173:PHE:O	0.45	2.42	14	1
2:H:141:MET:HE1	2:H:169:GLY:HA3	0.45	1.88	15	2
2:H:151:ILE:CG2	2:H:171:ILE:CG2	0.45	2.94	19	1
2:H:87:TYR:HB2	2:H:93:ALA:HB2	0.45	1.87	20	1
2:H:58:LEU:C	2:H:58:LEU:HD13	0.45	2.37	12	7
2:H:175:LYS:HG3	2:H:178:GLU:HB2	0.45	1.89	4	2
2:H:45:TYR:N	2:H:81:GLY:O	0.45	2.49	5	1
1:R:3:U:N3	2:H:109:THR:HG22	0.45	2.26	8	1
2:H:97:ILE:HG23	2:H:112:VAL:HB	0.45	1.86	8	1
2:H:43:VAL:CG1	2:H:110:ILE:HG22	0.45	2.40	11	2
1:R:1:A:OP2	2:H:166:ARG:HD3	0.45	2.11	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:50:MET:HE3	2:H:54:GLU:HB3	0.45	1.87	14	1
2:H:157:LEU:HD23	2:H:157:LEU:H	0.45	1.70	13	2
2:H:158:LEU:HB2	2:H:165:SER:HA	0.45	1.87	16	1
1:R:7:U:H4'	2:H:82:TYR:OH	0.45	2.11	18	3
2:H:125:ALA:HB3	2:H:173:PHE:C	0.45	2.37	6	2
1:R:3:U:C4	2:H:45:TYR:CE2	0.45	3.04	21	2
2:H:102:GLY:N	2:H:111:LYS:HG2	0.45	2.27	14	2
1:R:7:U:H4'	2:H:82:TYR:HH	0.45	1.72	17	1
2:H:157:LEU:HD11	2:H:166:ARG:HG2	0.45	1.88	17	1
2:H:59:PHE:HE2	2:H:100:LEU:HD13	0.45	1.70	1	1
2:H:168:VAL:HG12	2:H:169:GLY:N	0.45	2.27	7	5
1:R:0:U:O3'	1:R:1:A:H2'	0.45	2.12	8	1
2:H:157:LEU:H	2:H:157:LEU:HD13	0.45	1.72	10	1
2:H:130:SER:OG	2:H:199:THR:HB	0.45	2.12	11	1
2:H:141:MET:HE1	2:H:155:ARG:O	0.45	2.11	11	1
2:H:127:LEU:CD1	2:H:179:ALA:HB1	0.45	2.40	18	1
2:H:43:VAL:HA	2:H:112:VAL:HA	0.45	1.89	20	1
2:H:46:LEU:HD23	2:H:110:ILE:HD12	0.45	1.89	20	1
2:H:46:LEU:HD13	2:H:70:LEU:HD11	0.45	1.87	3	1
2:H:154:SER:CB	2:H:171:ILE:HD13	0.45	2.42	4	1
1:R:2:U:O4'	2:H:157:LEU:HG	0.45	2.11	16	1
2:H:129:VAL:HA	2:H:199:THR:O	0.45	2.12	17	1
2:H:151:ILE:HG12	2:H:171:ILE:CG2	0.44	2.42	7	1
2:H:159:ASP:CG	2:H:160:GLN:N	0.44	2.75	8	1
2:H:46:LEU:HD23	2:H:110:ILE:HD11	0.44	1.88	14	1
1:R:5:A:H4'	1:R:6:U:OP2	0.44	2.12	4	1
2:H:101:ASN:OD1	2:H:111:LYS:NZ	0.44	2.39	6	2
2:H:127:LEU:HD21	2:H:183:ILE:CD1	0.44	2.34	9	1
2:H:97:ILE:O	2:H:101:ASN:ND2	0.44	2.49	12	1
2:H:90:PRO:HA	2:H:93:ALA:HB3	0.44	1.88	19	1
1:R:4:U:H3'	1:R:4:U:O2	0.44	2.13	4	1
1:R:8:U:H6	1:R:8:U:O5'	0.44	1.96	6	1
2:H:157:LEU:HD12	2:H:166:ARG:CB	0.44	2.42	11	1
1:R:2:U:O5'	2:H:157:LEU:HG	0.44	2.12	14	1
2:H:153:THR:OG1	2:H:172:ARG:HB3	0.44	2.12	14	1
2:H:71:VAL:HG21	2:H:82:TYR:HE2	0.44	1.69	17	1
2:H:56:LYS:O	2:H:60:GLY:N	0.44	2.47	2	1
2:H:132:LEU:HB3	2:H:136:MET:HG2	0.44	1.89	19	2
1:R:1:A:N1	2:H:204:ASN:CB	0.44	2.79	21	2
2:H:157:LEU:HD12	2:H:170:PHE:CZ	0.44	2.48	14	1
2:H:92:ASP:OD1	2:H:95:LYS:NZ	0.44	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:2:U:O5'	1:R:2:U:H6	0.44	1.95	18	2
2:H:151:ILE:HD13	2:H:171:ILE:HG23	0.44	1.90	18	3
2:H:162:THR:OG1	2:H:163:GLY:N	0.44	2.51	8	1
2:H:157:LEU:CD1	2:H:157:LEU:N	0.44	2.81	10	1
2:H:157:LEU:HD12	2:H:166:ARG:HE	0.44	1.73	15	1
2:H:69:LYS:HB3	2:H:84:PHE:CD2	0.44	2.48	8	2
1:R:6:U:H5	2:H:152:ILE:HG22	0.44	1.70	14	3
1:R:8:U:O4'	2:H:71:VAL:HG13	0.44	2.12	18	1
2:H:141:MET:HB3	2:H:171:ILE:HD11	0.44	1.89	18	1
2:H:97:ILE:HG12	2:H:112:VAL:CG1	0.44	2.43	8	1
2:H:103:LEU:O	2:H:110:ILE:N	0.44	2.51	10	2
2:H:79:SER:OG	2:H:80:LEU:N	0.44	2.49	20	1
2:H:97:ILE:HG23	2:H:101:ASN:HB2	0.44	1.90	7	1
2:H:100:LEU:HA	2:H:103:LEU:CD1	0.44	2.43	18	1
1:R:2:U:C1'	2:H:170:PHE:CE2	0.43	3.01	16	2
2:H:127:LEU:HD11	2:H:179:ALA:CB	0.43	2.40	18	1
2:H:151:ILE:HG21	2:H:171:ILE:HG23	0.43	1.89	19	1
1:R:6:U:OP2	2:H:45:TYR:CD1	0.43	2.71	8	1
2:H:82:TYR:CD2	2:H:84:PHE:HE1	0.43	2.31	8	1
2:H:95:LYS:HG3	2:H:96:ALA:N	0.43	2.28	10	1
2:H:68:CYS:HA	2:H:84:PHE:O	0.43	2.12	7	3
2:H:128:TYR:HE1	2:H:168:VAL:HG21	0.43	1.73	7	1
2:H:44:ASN:C	2:H:45:TYR:CD1	0.43	2.96	13	1
1:R:7:U:C4'	1:R:8:U:OP1	0.43	2.66	19	1
1:R:8:U:C1'	1:R:9:U:OP1	0.43	2.66	3	1
1:R:3:U:C4	2:H:45:TYR:CE1	0.43	3.06	13	1
1:R:3:U:H2'	2:H:45:TYR:CD1	0.43	2.48	16	1
2:H:110:ILE:O	2:H:110:ILE:HG23	0.43	2.12	16	1
2:H:132:LEU:HB3	2:H:136:MET:CG	0.43	2.44	19	1
1:R:5:A:O2'	2:H:82:TYR:OH	0.43	2.37	2	1
2:H:45:TYR:CD1	2:H:108:LYS:HG2	0.43	2.49	7	1
2:H:47:PRO:HG2	2:H:50:MET:HB2	0.43	1.90	10	1
2:H:105:LEU:CD1	2:H:110:ILE:HG13	0.43	2.44	10	1
1:R:4:U:C5	1:R:5:A:N7	0.43	2.87	13	1
2:H:128:TYR:O	2:H:200:VAL:HA	0.43	2.13	1	1
2:H:103:LEU:N	2:H:110:ILE:O	0.43	2.49	20	1
2:H:142:GLU:O	2:H:146:SER:HB2	0.43	2.13	5	4
2:H:109:THR:O	2:H:110:ILE:C	0.43	2.60	3	1
2:H:140:GLU:O	2:H:143:GLN:HG3	0.43	2.14	19	3
2:H:132:LEU:CD1	2:H:169:GLY:HA3	0.43	2.43	8	1
2:H:180:GLU:HA	2:H:183:ILE:HD12	0.43	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:129:VAL:CG1	2:H:200:VAL:HB	0.43	2.42	21	1
1:R:1:A:H4'	2:H:157:LEU:CD2	0.43	2.44	17	6
1:R:6:U:N3	2:H:113:SER:HB2	0.43	2.29	3	1
1:R:0:U:C6	1:R:0:U:OP3	0.43	2.72	5	1
1:R:9:U:OP2	2:H:71:VAL:HG13	0.43	2.13	10	1
2:H:118:SER:O	2:H:119:SER:CB	0.43	2.66	15	1
1:R:8:U:H3'	1:R:9:U:O3'	0.43	2.13	17	1
2:H:66:GLU:HB3	2:H:86:ASN:O	0.43	2.14	17	1
2:H:165:SER:C	2:H:166:ARG:HD3	0.43	2.39	20	2
2:H:141:MET:HE2	2:H:171:ILE:CD1	0.43	2.35	2	1
1:R:1:A:OP1	2:H:166:ARG:HD2	0.43	2.13	5	1
2:H:47:PRO:HG2	2:H:50:MET:HB3	0.43	1.90	14	3
1:R:0:U:H3'	1:R:0:U:O2	0.43	2.13	20	1
2:H:44:ASN:HA	2:H:82:TYR:CB	0.42	2.44	1	1
1:R:1:A:P	1:R:1:A:H3'	0.42	2.54	5	1
1:R:6:U:C2'	1:R:7:U:O5'	0.42	2.66	11	2
2:H:179:ALA:HB3	2:H:202:PHE:CZ	0.42	2.48	8	2
2:H:156:ILE:HA	2:H:168:VAL:O	0.42	2.14	16	1
1:R:3:U:N3	2:H:45:TYR:CD2	0.42	2.87	21	1
2:H:128:TYR:O	2:H:201:LYS:N	0.42	2.50	1	1
2:H:106:GLN:O	2:H:107:THR:CG2	0.42	2.62	2	1
2:H:183:ILE:HG23	2:H:201:LYS:HA	0.42	1.90	16	1
2:H:126:ASN:HB2	2:H:172:ARG:CZ	0.42	2.44	20	1
2:H:157:LEU:HD11	2:H:170:PHE:CZ	0.42	2.49	7	1
2:H:46:LEU:HD11	2:H:83:GLY:HA3	0.42	1.90	19	1
1:R:8:U:C5	2:H:84:PHE:CD1	0.42	3.07	2	1
1:R:8:U:C5	2:H:42:ILE:HD12	0.42	2.49	3	2
2:H:166:ARG:N	2:H:166:ARG:HD2	0.42	2.29	13	1
2:H:70:LEU:HD23	2:H:71:VAL:N	0.42	2.29	20	1
1:R:0:U:HO2'	1:R:1:A:P	0.42	2.38	5	1
1:R:5:A:N3	2:H:80:LEU:CD1	0.42	2.74	7	1
1:R:2:U:O4'	2:H:157:LEU:HB3	0.42	2.13	8	1
2:H:138:GLN:HB3	2:H:155:ARG:HA	0.42	1.91	19	1
2:H:64:ASP:C	2:H:65:ILE:HG13	0.42	2.39	20	1
2:H:181:GLU:OE1	2:H:184:LYS:NZ	0.42	2.43	5	2
1:R:1:A:O5'	2:H:157:LEU:HD11	0.42	2.14	3	1
2:H:71:VAL:CG2	2:H:84:PHE:CE2	0.42	3.02	8	2
2:H:138:GLN:HB2	2:H:155:ARG:HA	0.42	1.91	19	1
2:H:127:LEU:HD22	2:H:183:ILE:CD1	0.42	2.33	1	1
2:H:69:LYS:HB3	2:H:84:PHE:HD2	0.42	1.74	3	3
2:H:71:VAL:HG11	2:H:82:TYR:HE1	0.42	1.74	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:41:LEU:O	2:H:85:VAL:N	0.42	2.50	8	1
2:H:157:LEU:CD1	2:H:157:LEU:H	0.42	2.28	14	1
1:R:8:U:OP1	2:H:71:VAL:CG1	0.42	2.67	15	1
2:H:62:ILE:CD1	2:H:100:LEU:HD21	0.42	2.45	5	1
2:H:132:LEU:HD12	2:H:169:GLY:N	0.42	2.29	5	1
2:H:155:ARG:O	2:H:170:PHE:N	0.42	2.46	6	2
2:H:134:LYS:HD2	2:H:135:THR:N	0.42	2.30	8	1
2:H:46:LEU:O	2:H:108:LYS:NZ	0.42	2.43	16	1
2:H:96:ALA:O	2:H:99:THR:HG22	0.42	2.15	20	1
2:H:128:TYR:HA	2:H:170:PHE:HD1	0.42	1.72	21	1
2:H:157:LEU:CD1	2:H:166:ARG:HG3	0.42	2.44	9	2
2:H:71:VAL:HG11	2:H:82:TYR:CZ	0.42	2.49	6	1
2:H:158:LEU:HA	2:H:166:ARG:HG3	0.42	1.92	10	1
2:H:141:MET:HE3	2:H:171:ILE:HD11	0.42	1.91	15	1
1:R:3:U:O2'	1:R:4:U:O5'	0.42	2.37	18	1
2:H:47:PRO:HA	2:H:108:LYS:CE	0.42	2.45	3	1
2:H:84:PHE:CD1	2:H:84:PHE:N	0.42	2.87	21	2
1:R:0:U:H4'	1:R:1:A:OP2	0.42	2.15	13	1
2:H:132:LEU:HD13	2:H:136:MET:HG2	0.42	1.90	18	1
2:H:43:VAL:O	2:H:83:GLY:N	0.41	2.47	3	1
1:R:5:A:OP2	2:H:172:ARG:HD2	0.41	2.15	8	1
2:H:139:LYS:NZ	2:H:142:GLU:OE1	0.41	2.51	8	1
2:H:69:LYS:HB3	2:H:84:PHE:HB2	0.41	1.91	13	2
2:H:127:LEU:HD23	2:H:127:LEU:N	0.41	2.30	16	1
2:H:43:VAL:HG21	2:H:59:PHE:CZ	0.41	2.50	3	1
1:R:3:U:O4	2:H:111:LYS:HE3	0.41	2.15	4	1
2:H:44:ASN:HA	2:H:82:TYR:HB3	0.41	1.92	18	2
2:H:145:PHE:HB3	2:H:171:ILE:HG21	0.41	1.91	16	1
2:H:175:LYS:HE3	2:H:178:GLU:CD	0.41	2.39	6	1
1:R:6:U:O4'	2:H:44:ASN:CB	0.41	2.68	7	1
2:H:80:LEU:HD23	2:H:82:TYR:OH	0.41	2.15	11	1
2:H:58:LEU:C	2:H:58:LEU:CD1	0.41	2.93	8	1
2:H:136:MET:CG	2:H:156:ILE:CD1	0.41	2.98	8	1
2:H:139:LYS:NZ	2:H:142:GLU:OE2	0.41	2.42	14	1
1:R:7:U:O2'	1:R:8:U:H5	0.41	1.99	15	1
2:H:130:SER:N	2:H:199:THR:O	0.41	2.48	17	1
2:H:129:VAL:N	2:H:169:GLY:O	0.41	2.49	19	1
2:H:130:SER:HA	2:H:168:VAL:HG13	0.41	1.92	19	2
2:H:130:SER:CA	2:H:168:VAL:HG13	0.41	2.45	19	1
2:H:157:LEU:O	2:H:166:ARG:HB2	0.41	2.15	10	2
1:R:6:U:O2	2:H:45:TYR:CE2	0.41	2.74	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:157:LEU:HD12	2:H:157:LEU:N	0.41	2.29	7	1
1:R:3:U:O4	2:H:111:LYS:HD2	0.41	2.15	8	1
1:R:2:U:C4'	2:H:157:LEU:HD13	0.41	2.45	12	1
2:H:105:LEU:HD11	2:H:110:ILE:HB	0.41	1.93	14	1
1:R:5:A:C6	2:H:79:SER:O	0.41	2.74	16	1
2:H:42:ILE:N	2:H:113:SER:O	0.41	2.52	6	1
2:H:186:LEU:C	2:H:198:ILE:HD11	0.41	2.41	6	1
1:R:3:U:H3	2:H:109:THR:HG22	0.41	1.76	8	1
2:H:43:VAL:HG22	2:H:112:VAL:CG2	0.41	2.40	13	1
2:H:105:LEU:HG	2:H:110:ILE:HD11	0.41	1.93	13	1
2:H:109:THR:HG22	2:H:109:THR:O	0.41	2.16	16	1
2:H:104:LYS:O	2:H:104:LYS:HG2	0.41	2.16	18	1
2:H:42:ILE:HG22	2:H:115:ALA:HB2	0.41	1.92	1	1
2:H:41:LEU:HD12	2:H:114:TYR:HA	0.41	1.93	3	1
1:R:2:U:C6	1:R:2:U:O5'	0.41	2.74	6	1
2:H:142:GLU:O	2:H:151:ILE:HD12	0.41	2.15	11	1
2:H:159:ASP:HB3	2:H:164:VAL:N	0.41	2.31	12	2
2:H:158:LEU:HD22	2:H:158:LEU:O	0.41	2.15	14	1
2:H:42:ILE:HD12	2:H:84:PHE:CE2	0.41	2.50	16	1
1:R:3:U:OP1	2:H:155:ARG:HD3	0.41	2.15	21	1
1:R:1:A:C4	2:H:128:TYR:CZ	0.41	3.08	7	1
2:H:95:LYS:O	2:H:95:LYS:HE3	0.41	2.15	9	1
1:R:6:U:O2	2:H:42:ILE:HD13	0.41	2.16	14	1
1:R:2:U:O4'	2:H:170:PHE:CE2	0.41	2.73	16	1
2:H:93:ALA:O	2:H:97:ILE:HG12	0.41	2.16	19	1
1:R:3:U:O2	2:H:109:THR:O	0.41	2.38	5	2
2:H:51:THR:HG22	2:H:54:GLU:OE1	0.41	2.16	5	1
1:R:6:U:H5	2:H:153:THR:HG23	0.41	1.75	14	1
2:H:127:LEU:HB2	2:H:171:ILE:O	0.41	2.16	14	1
2:H:158:LEU:C	2:H:158:LEU:CD2	0.41	2.92	14	1
2:H:71:VAL:HG11	2:H:82:TYR:CE1	0.41	2.51	19	1
2:H:70:LEU:HG	2:H:82:TYR:O	0.41	2.15	20	1
1:R:6:U:H5''	2:H:45:TYR:CE2	0.41	2.51	21	1
2:H:180:GLU:OE2	2:H:184:LYS:NZ	0.41	2.43	1	1
2:H:129:VAL:HA	2:H:200:VAL:HA	0.41	1.92	4	1
2:H:138:GLN:OE1	2:H:155:ARG:NH2	0.41	2.51	4	2
1:R:3:U:O2	2:H:45:TYR:CD2	0.41	2.74	7	1
2:H:149:GLY:HA3	2:H:173:PHE:CE2	0.40	2.51	5	1
2:H:176:ARG:HG3	2:H:177:ILE:N	0.40	2.30	5	1
1:R:9:U:OP1	2:H:71:VAL:HG21	0.40	2.16	8	1
2:H:141:MET:SD	2:H:171:ILE:HD11	0.40	2.56	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:100:LEU:O	2:H:111:LYS:HA	0.40	2.16	11	1
2:H:102:GLY:HA2	2:H:111:LYS:HE2	0.40	1.93	14	1
1:R:7:U:C2	2:H:115:ALA:HB1	0.40	2.51	15	1
2:H:176:ARG:HG2	2:H:202:PHE:CE1	0.40	2.51	17	1
2:H:165:SER:C	2:H:166:ARG:CD	0.40	2.95	1	1
1:R:1:A:H5'	2:H:168:VAL:CG2	0.40	2.47	7	1
2:H:101:ASN:OD1	2:H:111:LYS:HE2	0.40	2.15	10	1
2:H:118:SER:O	2:H:119:SER:HB3	0.40	2.16	15	1
1:R:0:U:O2	1:R:0:U:H3'	0.40	2.16	16	1
2:H:46:LEU:HD12	2:H:83:GLY:N	0.40	2.31	17	1
2:H:66:GLU:O	2:H:67:SER:HB2	0.40	2.16	8	1
2:H:165:SER:O	2:H:166:ARG:NE	0.40	2.38	11	1
1:R:1:A:N1	2:H:128:TYR:CD2	0.40	2.89	12	1
1:R:6:U:C2	2:H:44:ASN:OD1	0.40	2.75	14	1
2:H:82:TYR:CE2	2:H:84:PHE:CZ	0.40	3.09	14	1
2:H:107:THR:O	2:H:108:LYS:HG3	0.40	2.16	16	1
2:H:157:LEU:O	2:H:157:LEU:CG	0.40	2.69	6	1
1:R:5:A:C4	2:H:80:LEU:HA	0.40	2.51	16	1
2:H:104:LYS:O	2:H:105:LEU:HG	0.40	2.17	17	1
2:H:45:TYR:CB	2:H:109:THR:O	0.40	2.69	19	1
2:H:202:PHE:O	2:H:203:ALA:C	0.40	2.65	2	1
2:H:58:LEU:HD13	2:H:58:LEU:C	0.40	2.41	3	1
2:H:187:ASN:OD1	2:H:201:LYS:NZ	0.40	2.52	5	1
1:R:8:U:C2	2:H:84:PHE:CD2	0.40	3.09	8	1
1:R:6:U:H4'	2:H:82:TYR:CE1	0.40	2.51	11	1
1:R:6:U:O2'	1:R:7:U:OP1	0.40	2.40	12	1
2:H:82:TYR:N	2:H:82:TYR:CD1	0.40	2.90	14	1
2:H:179:ALA:HB3	2:H:202:PHE:HZ	0.40	1.77	18	1
2:H:41:LEU:CD1	2:H:114:TYR:HA	0.40	2.47	19	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	
2	H	147/174 (84%)	116±13 (79±9%)	22±3 (15±2%)	5±2 (3±1%)	4	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3010/3654 (82%)	2437 (81%)	468 (16%)	105 (3%)	4	33

All 28 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	H	102	GLY	15
2	H	198	ILE	11
2	H	150	ARG	10
2	H	81	GLY	9
2	H	161	ALA	9
2	H	149	GLY	7
2	H	79	SER	6
2	H	47	PRO	6
2	H	99	THR	4
2	H	160	GLN	3
2	H	187	ASN	3
2	H	119	SER	3
2	H	118	SER	2
2	H	117	PRO	2
2	H	124	ASP	2
2	H	107	THR	1
2	H	110	ILE	1
2	H	48	GLN	1
2	H	49	ASN	1
2	H	39	THR	1
2	H	90	PRO	1
2	H	38	LYS	1
2	H	106	GLN	1
2	H	155	ARG	1
2	H	204	ASN	1
2	H	65	ILE	1
2	H	101	ASN	1
2	H	203	ALA	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	
2	H	127/149 (85%)	87±26 (69±20%)	24±9 (19±7%)	3	35
All	All	2333/3129 (75%)	1835 (79%)	498 (21%)	3	31

All 80 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)
2	H	95	LYS	15
2	H	100	LEU	15
2	H	143	GLN	15
2	H	144	LEU	13
2	H	82	TYR	13
2	H	38	LYS	12
2	H	158	LEU	12
2	H	175	LYS	12
2	H	184	LYS	12
2	H	142	GLU	11
2	H	155	ARG	11
2	H	200	VAL	11
2	H	201	LYS	11
2	H	44	ASN	10
2	H	116	ARG	10
2	H	134	LYS	10
2	H	139	LYS	10
2	H	165	SER	10
2	H	111	LYS	10
2	H	104	LYS	9
2	H	126	ASN	9
2	H	66	GLU	9
2	H	98	ASN	8
2	H	99	THR	8
2	H	108	LYS	8
2	H	157	LEU	8
2	H	160	GLN	8
2	H	137	SER	8
2	H	61	SER	7
2	H	64	ASP	7
2	H	69	LYS	7
2	H	140	GLU	7
2	H	150	ARG	7
2	H	138	GLN	7
2	H	88	SER	7
2	H	176	ARG	7

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Mol	Chain	Res	Type	Models (Total)
2	H	118	SER	6
2	H	178	GLU	6
2	H	180	GLU	6
2	H	187	ASN	6
2	H	166	ARG	6
2	H	39	THR	6
2	H	52	GLN	6
2	H	89	ASP	5
2	H	110	ILE	5
2	H	124	ASP	5
2	H	181	GLU	5
2	H	136	MET	5
2	H	54	GLU	4
2	H	42	ILE	4
2	H	48	GLN	4
2	H	141	MET	4
2	H	151	ILE	4
2	H	198	ILE	4
2	H	79	SER	4
2	H	86	ASN	4
2	H	172	ARG	3
2	H	57	SER	3
2	H	146	SER	3
2	H	41	LEU	3
2	H	91	ASN	3
2	H	58	LEU	3
2	H	50	MET	2
2	H	56	LYS	2
2	H	92	ASP	2
2	H	40	ASN	2
2	H	67	SER	2
2	H	101	ASN	2
2	H	119	SER	2
2	H	106	GLN	2
2	H	53	ASP	2
2	H	156	ILE	1
2	H	80	LEU	1
2	H	46	LEU	1
2	H	49	ASN	1
2	H	204	ASN	1
2	H	113	SER	1
2	H	154	SER	1

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Mol	Chain	Res	Type	Models (Total)
2	H	132	LEU	1
2	H	109	THR	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	R	9/10 (90%)	8±0 (89±0%)	2±1 (19±10%)	0.01±0.00
All	All	193/210 (92%)	168 (87%)	36 (19%)	0.01

The overall RNA backbone suiteness is 0.01.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	R	1	A	21
1	R	2	U	21
1	R	3	U	21
1	R	4	U	21
1	R	5	A	21
1	R	6	U	21
1	R	8	U	21
1	R	9	U	21

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	R	5	A	17
1	R	6	U	5
1	R	8	U	4
1	R	0	U	4
1	R	4	U	2
1	R	7	U	2
1	R	2	U	2

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided