



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:33 PM UTC

PDB ID : 1K1G / pdb_00001k1g
Title : STRUCTURAL BASIS FOR RECOGNITION OF THE INTRON BRANCH SITE RNA BY SPLICING FACTOR 1
Authors : Liu, Z.; Luyten, I.; Bottomley, M.J.; Messias, A.C.; Houngninou-Molango, S.; Sprangers, R.; Zanier, K.; Kramer, A.; Sattler, M.
Deposited on : 2001-09-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

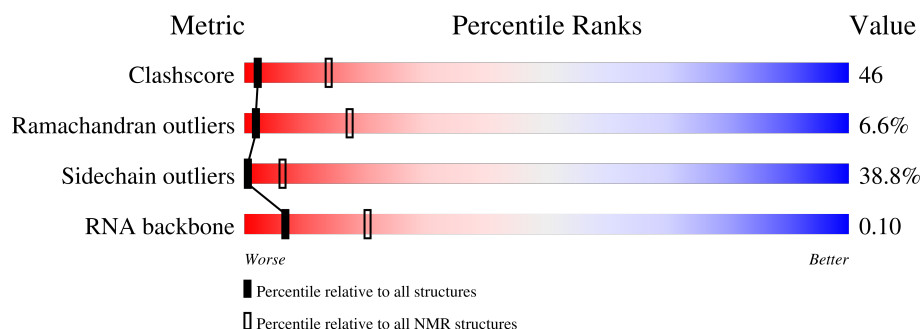
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	B	11	27% 73%
2	A	131	29% 36% 20% • 8% 7%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:134-A:184, A:195-A:255 (112)	0.67	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 8
2	1, 6
Single-model clusters	2; 7; 9; 10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2308 atoms, of which 1122 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms						Trace
1	B	11	Total	C	H	N	O	P	0
			349	105	120	42	72	10	

- Molecule 2 is a protein called SF1-Bo isoform.

Mol	Chain	Residues	Atoms						Trace
2	A	122	Total	C	H	N	O	S	0
			1959	591	1002	178	182	6	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	LYS	cloning artifact	UNP Q15637
A	131	ALA	PRO	cloning artifact	UNP Q15637
A	132	MET	PRO	cloning artifact	UNP Q15637

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

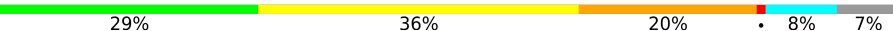
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

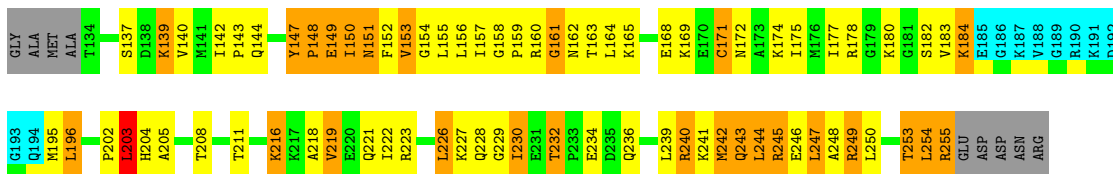
- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

Chain A: 



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

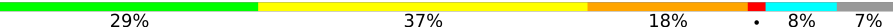
4.2.1 Score per residue for model 1

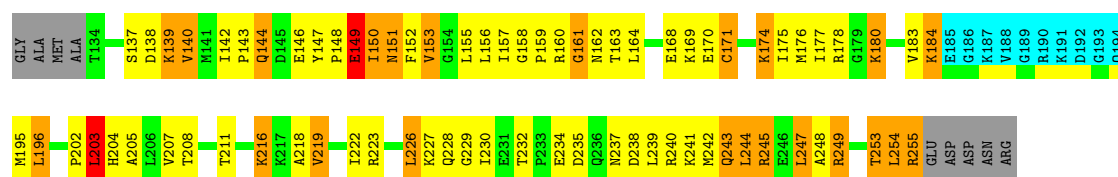
- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

Chain A: 

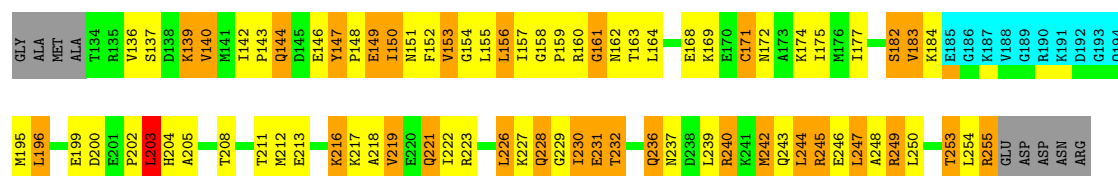
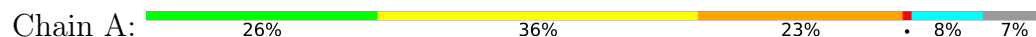


4.2.2 Score per residue for model 2

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform

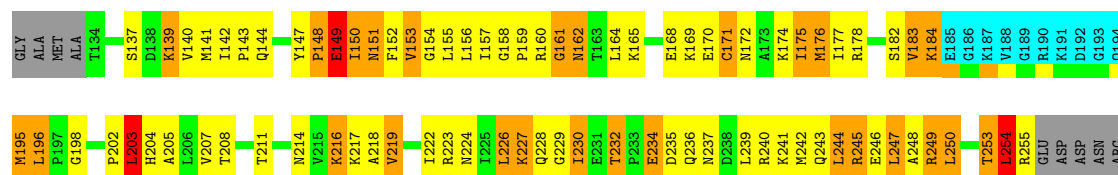
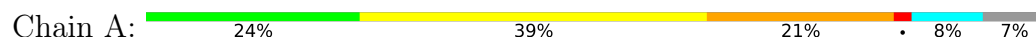


4.2.3 Score per residue for model 3

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform



4.2.4 Score per residue for model 4

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 27% 73%

U501
A502
U503
A504
C505
U506
A507
A508
C509
A510
A511

- Molecule 2: SF1-Bo isoform

Chain A: 28% 38% 18% 8% 7%

GLY
ALA
MET
ALA
T134
R135
V136
S137
D138
K139
V140
V141
I142
Y147
P148
E149
I150
M151
F152
V153
G154
L155
L156
I157
G158
P159
R160
G161
N162
T163
L164
K165
E168
K169
E170
G171
N172
K174
I177
R178
G179
K180
G181
S182
V183
K184
E185
G186
K187
V188
G189
R190
K191
D192
G193
Q194
M195
L196
E199
D200
E201
P202
L203
A205
T208
T211
R212
E213
N214
V215
K216
K217
K218
V219
I222
R223
N224
L225
L226
K227
Q228
G229
T230
E231
T232
P233
E234
D235
Q236
R240
K241
Q242
Q243
L244
R245
E246
L247
A248
R249
L250
T253
L254
R255
GLU
ASP
ASP
ASN
ARG

4.2.5 Score per residue for model 5

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 9% 18% 73%

U501
A502
U503
A504
C505
U506
A507
A508
C509
A510
A511

- Molecule 2: SF1-Bo isoform

Chain A: 25% 38% 21% 8% 7%

GLY
ALA
MET
ALA
T134
S137
D138
K139
V140
M141
I142
P143
Q144
Y147
P148
E149
I150
M151
F152
V153
G154
L155
L156
I157
G158
P159
R160
G161
N162
T163
L164
K165
I167
E168
K169
E170
G171
N172
K174
I177
R178
G179
K180
V183
K184
E185
G186
K187
V188
G189
R190
K191
D192
G193
L194
M195
L196
P197
G198
E199
D200
E201
P202
L203
R204
A205
L206
V207
T208
A209
T210
N211
K212
E213
R214
R215
R216
V219
I222
R223
L226
K227
Q228
G229
T230
E231
T232
R235
Q236
L239
R240
K241
N242
Q243
L244
R245
E246
L247
A248
R249
L250
N251
T253
L254
R255
GLU
ASP
ASP

4.2.6 Score per residue for model 6

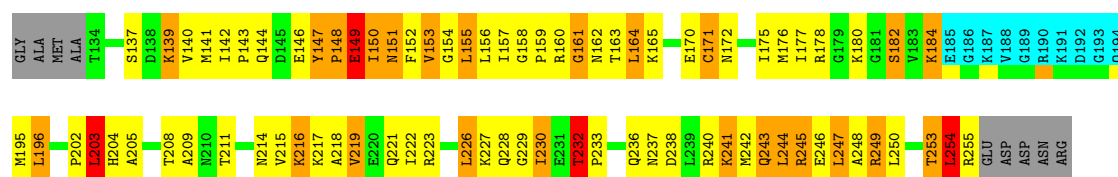
- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 27% 73%

U501
A502
U503
A504
C505
U506
A507
A508
C509
A510
A511

- Molecule 2: SF1-Bo isoform

Chain A: 25% 39% 18% 8% 7%

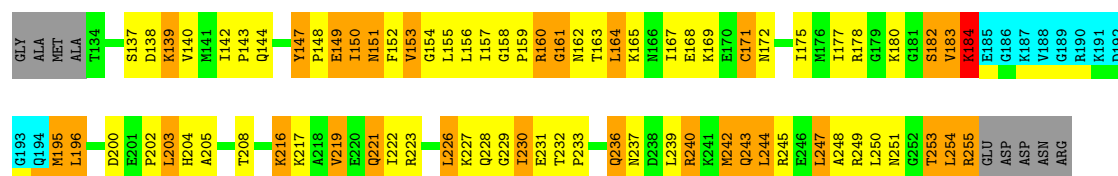
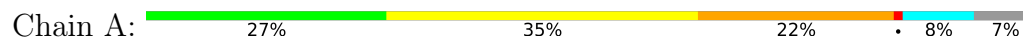


4.2.7 Score per residue for model 7

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform

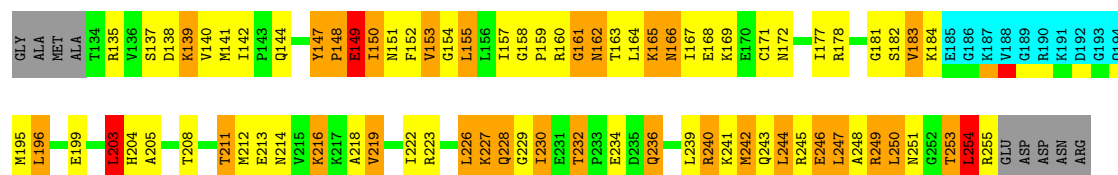
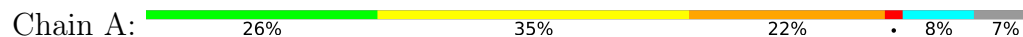


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform



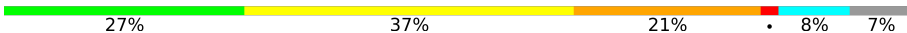
4.2.9 Score per residue for model 9

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

Chain A: 



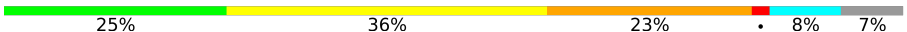
4.2.10 Score per residue for model 10

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

Chain A: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained molecular dynamics, simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *10 lowest energy structures consistent with experimental distance and dihedral angle restraints*.

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

Software name	Classification	Version
ARIA/CNS	structure solution	1.0
ARIA/CNS	refinement	1.0

No chemical shift data was provided.

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	B	229	120	120	27±3
2	A	883	927	925	90±6
All	All	11120	10470	10450	1001

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:507:A:C2	2:A:184:LYS:HG3	0.81	2.11	9	1
2:A:159:PRO:HD3	2:A:247:LEU:HB2	0.79	1.53	2	9
1:B:502:A:H2'	2:A:255:ARG:HA	0.75	1.58	8	7
2:A:151:ASN:HB2	2:A:155:LEU:HG	0.75	1.58	3	6
2:A:155:LEU:HD22	2:A:243:GLN:HB3	0.73	1.60	10	10
2:A:245:ARG:HD2	2:A:249:ARG:HB2	0.73	1.58	9	4
2:A:219:VAL:HA	2:A:222:ILE:HD12	0.72	1.61	4	10
2:A:153:VAL:HG23	2:A:177:ILE:HD13	0.72	1.61	3	10
2:A:142:ILE:HG13	2:A:226:LEU:HG	0.72	1.62	2	5
2:A:143:PRO:HD3	2:A:226:LEU:HD11	0.71	1.61	2	4
2:A:254:LEU:HD22	2:A:255:ARG:H	0.70	1.46	9	6
2:A:245:ARG:HD3	2:A:249:ARG:HB2	0.70	1.64	1	3
2:A:254:LEU:HD22	2:A:255:ARG:N	0.68	2.01	10	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:508:A:H2'	1:B:509:C:O4'	0.68	1.88	6	10
2:A:195:MET:HE3	2:A:196:LEU:HD23	0.68	1.66	6	2
1:B:510:A:H2'	1:B:511:A:H3'	0.68	1.66	5	3
1:B:506:U:O4	2:A:151:ASN:HB3	0.68	1.89	7	3
1:B:510:A:H4'	2:A:176:MET:HE2	0.67	1.66	3	1
2:A:245:ARG:HG2	2:A:254:LEU:HD23	0.67	1.66	7	9
2:A:228:GLN:HB3	2:A:232:THR:HB	0.67	1.65	9	6
1:B:506:U:C2	2:A:247:LEU:HD22	0.67	2.25	7	10
1:B:505:C:C2	2:A:244:LEU:HD11	0.66	2.25	2	10
2:A:139:LYS:HG3	2:A:204:HIS:HB2	0.66	1.68	8	9
1:B:508:A:H62	2:A:183:VAL:HG23	0.66	1.50	2	2
2:A:245:ARG:HD3	2:A:249:ARG:HB3	0.66	1.66	2	2
2:A:150:ILE:HD12	2:A:230:ILE:HD11	0.65	1.67	5	3
2:A:236:GLN:HB2	2:A:240:ARG:HB2	0.65	1.66	2	2
2:A:151:ASN:ND2	2:A:155:LEU:HD11	0.65	2.06	6	5
1:B:507:A:C4	2:A:184:LYS:HD3	0.64	2.27	3	2
1:B:505:C:H4'	1:B:506:U:O5'	0.64	1.92	8	4
2:A:236:GLN:HB2	2:A:239:LEU:HD12	0.63	1.70	8	1
2:A:157:ILE:HA	2:A:164:LEU:HG	0.63	1.70	10	10
2:A:142:ILE:HG13	2:A:226:LEU:HD11	0.63	1.69	5	4
2:A:140:VAL:CG1	2:A:205:ALA:HB3	0.62	2.24	9	9
2:A:161:GLY:HA3	2:A:164:LEU:HD12	0.62	1.69	3	10
2:A:147:TYR:CB	2:A:150:ILE:HD11	0.62	2.24	2	5
2:A:147:TYR:HB2	2:A:150:ILE:HD11	0.62	1.70	7	5
1:B:506:U:O2	2:A:247:LEU:HD22	0.62	1.93	3	10
2:A:151:ASN:O	2:A:155:LEU:HG	0.62	1.93	1	10
2:A:232:THR:HG21	2:A:240:ARG:HB3	0.62	1.70	2	1
2:A:151:ASN:ND2	2:A:155:LEU:HD21	0.62	2.09	8	2
2:A:242:MET:O	2:A:242:MET:HE2	0.62	1.95	10	2
2:A:157:ILE:HG23	2:A:164:LEU:HD11	0.62	1.70	4	10
2:A:242:MET:O	2:A:242:MET:HE3	0.61	1.96	3	6
1:B:507:A:H4'	1:B:508:A:O5'	0.61	1.95	9	10
2:A:147:TYR:HB3	2:A:150:ILE:HD11	0.61	1.73	8	4
2:A:177:ILE:HG22	2:A:182:SER:HB3	0.60	1.74	2	3
2:A:246:GLU:HG3	2:A:247:LEU:N	0.60	2.10	8	4
1:B:509:C:H2'	1:B:510:A:O4'	0.60	1.97	1	10
2:A:221:GLN:HG3	2:A:222:ILE:N	0.60	2.10	2	3
2:A:144:GLN:HA	2:A:147:TYR:O	0.59	1.97	1	9
1:B:507:A:H2'	2:A:184:LYS:HB2	0.59	1.73	2	7
2:A:244:LEU:HD23	2:A:247:LEU:CD2	0.59	2.27	10	10
2:A:151:ASN:HB2	2:A:155:LEU:CG	0.59	2.28	3	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:157:ILE:HG12	2:A:164:LEU:HD11	0.58	1.75	10	6
2:A:247:LEU:HG	2:A:248:ALA:N	0.58	2.13	9	9
2:A:248:ALA:HB1	2:A:253:THR:C	0.58	2.23	6	10
2:A:143:PRO:HD2	2:A:226:LEU:HD21	0.58	1.76	6	3
2:A:152:PHE:HE1	2:A:229:GLY:HA3	0.58	1.59	2	6
1:B:511:A:N6	2:A:178:ARG:HA	0.57	2.13	5	4
2:A:216:LYS:O	2:A:219:VAL:HG12	0.57	1.99	10	9
2:A:151:ASN:OD1	2:A:155:LEU:HD11	0.57	2.00	3	1
2:A:157:ILE:HG22	2:A:158:GLY:O	0.57	2.00	8	10
1:B:511:A:O2'	2:A:195:MET:HE1	0.57	2.00	6	6
1:B:507:A:N6	2:A:153:VAL:HG13	0.56	2.15	9	9
2:A:232:THR:OG1	2:A:237:ASN:HA	0.56	1.99	7	1
1:B:507:A:H2'	2:A:184:LYS:CB	0.56	2.30	3	2
1:B:504:A:O2'	2:A:244:LEU:HD22	0.56	2.00	2	10
2:A:164:LEU:HA	2:A:175:ILE:HG13	0.56	1.77	3	5
2:A:152:PHE:HB3	2:A:226:LEU:HG	0.56	1.76	5	2
1:B:502:A:H4'	1:B:503:U:H5	0.56	1.61	3	3
1:B:504:A:N7	2:A:255:ARG:HD2	0.55	2.15	7	1
2:A:228:GLN:HB2	2:A:232:THR:HB	0.55	1.77	8	1
2:A:177:ILE:HA	2:A:205:ALA:HA	0.55	1.77	7	9
2:A:219:VAL:O	2:A:223:ARG:HG2	0.55	2.02	7	10
2:A:157:ILE:HA	2:A:164:LEU:CG	0.55	2.31	10	8
1:B:508:A:N7	2:A:183:VAL:HG12	0.55	2.17	9	2
2:A:159:PRO:HD2	2:A:162:ASN:HB2	0.55	1.78	7	7
2:A:254:LEU:C	2:A:254:LEU:HD22	0.55	2.27	3	4
1:B:510:A:H2'	1:B:511:A:H5''	0.55	1.80	3	1
2:A:248:ALA:HB1	2:A:253:THR:O	0.54	2.02	4	6
1:B:506:U:C4	2:A:154:GLY:HA3	0.54	2.37	3	9
2:A:151:ASN:HD22	2:A:155:LEU:HD21	0.54	1.60	9	2
2:A:155:LEU:HD13	2:A:243:GLN:CB	0.54	2.33	6	10
2:A:242:MET:O	2:A:245:ARG:HB2	0.54	2.03	10	1
1:B:511:A:H61	2:A:178:ARG:HA	0.54	1.63	3	2
2:A:152:PHE:CE1	2:A:229:GLY:HA3	0.54	2.38	2	3
2:A:157:ILE:HG12	2:A:164:LEU:HD21	0.54	1.80	4	6
2:A:162:ASN:HD22	2:A:250:LEU:HD13	0.54	1.61	4	1
1:B:505:C:H5''	1:B:506:U:H5'	0.54	1.80	1	2
2:A:244:LEU:HD23	2:A:247:LEU:HD23	0.54	1.80	8	10
1:B:510:A:N3	1:B:511:A:H8	0.53	2.01	5	6
2:A:152:PHE:O	2:A:156:LEU:HD23	0.53	2.03	4	2
2:A:142:ILE:HA	2:A:226:LEU:HD11	0.53	1.81	8	2
2:A:207:VAL:HG21	2:A:222:ILE:HD13	0.53	1.80	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:142:ILE:HB	2:A:203:LEU:HB3	0.53	1.79	4	7
2:A:195:MET:HE2	2:A:196:LEU:HD23	0.53	1.79	1	3
2:A:230:ILE:O	2:A:240:ARG:HB2	0.53	2.03	8	3
2:A:140:VAL:HG12	2:A:205:ALA:HB3	0.52	1.82	6	6
1:B:510:A:C2	1:B:511:A:H2'	0.52	2.39	3	4
2:A:139:LYS:HG2	2:A:204:HIS:HB2	0.52	1.82	9	1
2:A:151:ASN:HD21	2:A:230:ILE:HG23	0.52	1.64	10	2
1:B:507:A:N3	2:A:184:LYS:HG2	0.52	2.20	6	2
1:B:507:A:C2	2:A:184:LYS:HD3	0.52	2.40	1	5
2:A:156:LEU:O	2:A:163:THR:HB	0.52	2.05	6	8
2:A:240:ARG:C	2:A:242:MET:H	0.52	2.13	2	2
2:A:171:CYS:SG	2:A:218:ALA:HB2	0.51	2.44	6	5
1:B:502:A:H4'	1:B:503:U:C5	0.51	2.40	8	3
2:A:175:ILE:HD12	2:A:175:ILE:N	0.51	2.20	6	1
2:A:211:THR:HG23	2:A:214:ASN:HB2	0.51	1.82	8	1
1:B:504:A:H4'	1:B:505:C:OP2	0.51	2.05	9	7
1:B:511:A:N7	2:A:183:VAL:HG11	0.51	2.21	8	7
1:B:508:A:N3	2:A:164:LEU:HD13	0.51	2.20	7	7
2:A:156:LEU:HD23	2:A:222:ILE:HG23	0.51	1.82	9	2
2:A:160:ARG:HD2	2:A:160:ARG:C	0.51	2.29	6	10
2:A:156:LEU:HD11	2:A:222:ILE:HG12	0.51	1.83	3	2
2:A:151:ASN:CG	2:A:155:LEU:HD11	0.51	2.30	8	2
2:A:155:LEU:HD22	2:A:243:GLN:CB	0.51	2.36	3	7
2:A:242:MET:HA	2:A:245:ARG:HB2	0.50	1.83	2	1
2:A:147:TYR:N	2:A:147:TYR:CD1	0.50	2.79	7	5
2:A:181:GLY:O	2:A:203:LEU:HD21	0.50	2.06	4	2
2:A:239:LEU:O	2:A:242:MET:HB3	0.50	2.06	3	6
2:A:151:ASN:O	2:A:152:PHE:C	0.50	2.55	2	8
1:B:508:A:H62	2:A:183:VAL:HG13	0.50	1.65	9	2
2:A:150:ILE:HG22	2:A:151:ASN:H	0.50	1.67	3	10
2:A:155:LEU:HD13	2:A:243:GLN:HB3	0.50	1.84	2	7
2:A:228:GLN:HA	2:A:232:THR:HA	0.50	1.84	9	5
2:A:245:ARG:NH1	2:A:249:ARG:HG2	0.50	2.21	10	1
1:B:508:A:O3'	2:A:160:ARG:HD3	0.50	2.07	4	10
2:A:149:GLU:O	2:A:150:ILE:C	0.50	2.54	10	10
1:B:511:A:N1	2:A:178:ARG:HG3	0.50	2.22	4	2
1:B:510:A:N3	1:B:511:A:H2'	0.49	2.22	9	3
2:A:223:ARG:HH11	2:A:223:ARG:HA	0.49	1.67	5	1
2:A:144:GLN:HG2	2:A:148:PRO:O	0.49	2.07	8	5
2:A:156:LEU:CA	2:A:225:ILE:HG21	0.49	2.37	4	1
2:A:142:ILE:HG13	2:A:226:LEU:CD1	0.49	2.37	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:207:VAL:HG12	2:A:215:VAL:HG23	0.49	1.84	5	1
2:A:157:ILE:HG23	2:A:161:GLY:HA2	0.49	1.84	1	6
1:B:502:A:H1'	1:B:503:U:OP1	0.49	2.08	4	2
1:B:511:A:C5	2:A:196:LEU:HD13	0.49	2.43	3	8
2:A:161:GLY:CA	2:A:164:LEU:HD12	0.49	2.38	1	9
2:A:156:LEU:O	2:A:156:LEU:HD12	0.49	2.08	2	2
1:B:505:C:N3	2:A:244:LEU:HD11	0.49	2.23	8	9
2:A:156:LEU:HD22	2:A:156:LEU:O	0.49	2.08	1	1
2:A:234:GLU:HA	2:A:237:ASN:HD22	0.48	1.68	3	1
2:A:232:THR:HG1	2:A:237:ASN:HA	0.48	1.68	7	1
2:A:156:LEU:CD1	2:A:222:ILE:HG23	0.48	2.38	10	1
2:A:226:LEU:O	2:A:227:LYS:C	0.48	2.56	9	10
2:A:223:ARG:O	2:A:227:LYS:HB2	0.48	2.08	9	2
1:B:505:C:H1'	1:B:506:U:C5	0.48	2.42	2	6
1:B:507:A:N3	2:A:184:LYS:HB2	0.48	2.23	3	2
1:B:507:A:N3	2:A:184:LYS:HD3	0.48	2.24	3	1
2:A:245:ARG:NH1	2:A:254:LEU:HG	0.48	2.24	3	1
2:A:136:VAL:HG11	2:A:211:THR:C	0.48	2.34	9	1
2:A:232:THR:HG23	2:A:240:ARG:HA	0.48	1.85	3	4
2:A:246:GLU:O	2:A:250:LEU:HB2	0.48	2.09	8	7
2:A:142:ILE:HD13	2:A:203:LEU:O	0.48	2.09	4	3
1:B:507:A:C2	2:A:184:LYS:HG2	0.48	2.44	6	1
2:A:177:ILE:HB	2:A:182:SER:HB3	0.48	1.85	9	1
2:A:230:ILE:HD13	2:A:230:ILE:N	0.47	2.24	2	4
2:A:149:GLU:O	2:A:150:ILE:O	0.47	2.32	6	6
1:B:511:A:N6	2:A:182:SER:HB2	0.47	2.24	9	1
1:B:507:A:H61	2:A:153:VAL:HG13	0.47	1.68	9	1
2:A:168:GLU:O	2:A:172:ASN:HA	0.47	2.09	7	5
1:B:508:A:H2'	1:B:509:C:C6	0.47	2.44	1	10
2:A:207:VAL:HG21	2:A:222:ILE:CD1	0.47	2.40	9	4
2:A:174:LYS:O	2:A:207:VAL:HA	0.47	2.09	3	3
2:A:151:ASN:O	2:A:155:LEU:N	0.47	2.48	3	9
2:A:230:ILE:HD13	2:A:230:ILE:H	0.47	1.69	3	1
1:B:504:A:O2'	2:A:244:LEU:HB3	0.47	2.10	4	3
1:B:502:A:H4'	1:B:503:U:OP2	0.47	2.09	10	1
2:A:245:ARG:HD3	2:A:254:LEU:HG	0.47	1.85	10	1
2:A:195:MET:O	2:A:195:MET:HG2	0.47	2.09	7	1
2:A:165:LYS:O	2:A:169:LYS:HB3	0.47	2.10	8	1
2:A:157:ILE:HA	2:A:164:LEU:CD2	0.46	2.40	1	6
1:B:502:A:H4'	1:B:503:U:C6	0.46	2.46	2	1
2:A:150:ILE:HD12	2:A:152:PHE:CZ	0.46	2.45	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:150:ILE:HG22	2:A:151:ASN:OD1	0.46	2.10	7	1
2:A:157:ILE:CG1	2:A:164:LEU:HD21	0.46	2.41	8	6
2:A:142:ILE:HG21	2:A:203:LEU:HD12	0.46	1.87	9	1
2:A:156:LEU:N	2:A:225:ILE:HG21	0.46	2.25	4	1
2:A:183:VAL:HG11	2:A:196:LEU:HD21	0.46	1.88	3	1
2:A:211:THR:HG23	2:A:214:ASN:H	0.46	1.71	6	3
2:A:228:GLN:O	2:A:229:GLY:C	0.45	2.60	8	1
2:A:184:LYS:CD	2:A:184:LYS:C	0.45	2.89	9	1
2:A:240:ARG:C	2:A:242:MET:N	0.45	2.75	2	1
1:B:506:U:O2'	1:B:507:A:H5'	0.45	2.11	2	1
2:A:149:GLU:HB3	2:A:203:LEU:HG	0.45	1.88	5	1
2:A:248:ALA:HB1	2:A:254:LEU:N	0.45	2.27	5	1
2:A:147:TYR:HE2	2:A:231:GLU:HB2	0.45	1.72	2	2
2:A:177:ILE:C	2:A:182:SER:HB3	0.45	2.37	10	2
2:A:139:LYS:HG3	2:A:204:HIS:CB	0.45	2.40	8	7
2:A:175:ILE:O	2:A:176:MET:HG3	0.45	2.12	3	2
2:A:243:GLN:O	2:A:246:GLU:HG2	0.45	2.12	4	1
1:B:505:C:OP1	2:A:253:THR:HG21	0.45	2.12	8	1
2:A:140:VAL:O	2:A:142:ILE:HD12	0.45	2.11	9	1
2:A:159:PRO:HD2	2:A:162:ASN:CG	0.45	2.37	4	1
2:A:223:ARG:HB3	2:A:227:LYS:HG3	0.45	1.88	5	2
1:B:502:A:H5'	1:B:503:U:H5	0.45	1.71	7	1
1:B:504:A:C5	2:A:255:ARG:HD2	0.45	2.47	8	1
2:A:155:LEU:HD22	2:A:243:GLN:C	0.45	2.36	3	2
1:B:507:A:H3'	2:A:184:LYS:HZ2	0.45	1.72	5	1
2:A:163:THR:O	2:A:167:ILE:HG12	0.45	2.12	10	3
2:A:221:GLN:O	2:A:224:ASN:HB3	0.45	2.12	10	1
2:A:226:LEU:HD13	2:A:227:LYS:N	0.44	2.27	2	2
1:B:505:C:C4'	1:B:506:U:H5'	0.44	2.42	1	2
1:B:501:U:H2'	1:B:503:U:C5	0.44	2.47	3	1
1:B:507:A:H2'	2:A:184:LYS:HD3	0.44	1.88	3	1
2:A:240:ARG:HG3	2:A:241:LYS:N	0.44	2.27	6	1
2:A:151:ASN:CB	2:A:155:LEU:HG	0.44	2.42	1	1
2:A:136:VAL:HG21	2:A:212:MET:HA	0.44	1.90	4	2
2:A:162:ASN:ND2	2:A:250:LEU:HD13	0.44	2.27	4	1
2:A:164:LEU:O	2:A:168:GLU:HG3	0.44	2.13	2	1
1:B:505:C:C5'	1:B:506:U:H5'	0.44	2.42	1	1
2:A:155:LEU:CD2	2:A:243:GLN:HB3	0.44	2.39	2	3
2:A:184:LYS:C	2:A:184:LYS:HD2	0.44	2.38	9	1
1:B:502:A:H4'	1:B:503:U:H6	0.43	1.71	2	1
2:A:155:LEU:HB3	2:A:243:GLN:HB3	0.43	1.89	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:156:LEU:CD2	2:A:222:ILE:HG23	0.43	2.42	9	2
1:B:502:A:H3'	2:A:255:ARG:NE	0.43	2.29	6	2
2:A:240:ARG:HD2	2:A:241:LYS:HD2	0.43	1.88	9	1
2:A:254:LEU:O	2:A:255:ARG:C	0.43	2.62	7	3
2:A:217:LYS:HG3	2:A:218:ALA:N	0.43	2.28	2	1
1:B:506:U:H6	1:B:506:U:OP2	0.43	1.96	8	2
2:A:254:LEU:HD22	2:A:255:ARG:HG2	0.43	1.90	5	2
1:B:501:U:O2'	1:B:503:U:H5'	0.43	2.13	6	2
2:A:157:ILE:HG23	2:A:164:LEU:CD1	0.43	2.43	10	5
2:A:240:ARG:HG3	2:A:241:LYS:H	0.43	1.72	9	2
2:A:254:LEU:O	2:A:255:ARG:HG3	0.43	2.13	8	1
2:A:232:THR:CG2	2:A:240:ARG:HA	0.43	2.44	5	3
2:A:139:LYS:CG	2:A:204:HIS:HB2	0.43	2.42	10	6
2:A:156:LEU:HD11	2:A:177:ILE:HD11	0.43	1.89	4	1
2:A:159:PRO:HD2	2:A:162:ASN:ND2	0.43	2.27	4	1
2:A:171:CYS:SG	2:A:217:LYS:HE2	0.43	2.53	6	3
2:A:151:ASN:O	2:A:154:GLY:N	0.43	2.51	5	3
2:A:166:ASN:O	2:A:169:LYS:HG2	0.43	2.14	8	1
1:B:507:A:H1'	1:B:508:A:C8	0.43	2.49	9	1
2:A:135:ARG:HH12	2:A:174:LYS:HD2	0.43	1.72	9	1
1:B:511:A:C6	2:A:196:LEU:HD13	0.43	2.49	5	1
2:A:209:ALA:HB3	2:A:215:VAL:HB	0.43	1.89	10	3
2:A:157:ILE:O	2:A:163:THR:N	0.43	2.52	8	2
2:A:156:LEU:O	2:A:156:LEU:HD22	0.42	2.14	9	1
2:A:212:MET:HA	2:A:215:VAL:HG12	0.42	1.90	10	2
2:A:151:ASN:HB3	2:A:155:LEU:HG	0.42	1.91	1	1
2:A:140:VAL:O	2:A:204:HIS:HA	0.42	2.14	2	1
2:A:254:LEU:C	2:A:254:LEU:CD2	0.42	2.92	3	2
2:A:254:LEU:HD13	2:A:255:ARG:H	0.42	1.75	3	1
2:A:230:ILE:H	2:A:230:ILE:HD13	0.42	1.74	5	1
2:A:147:TYR:CD1	2:A:147:TYR:N	0.42	2.86	8	2
2:A:146:GLU:HB3	2:A:147:TYR:CD1	0.42	2.50	6	1
1:B:508:A:H62	2:A:183:VAL:HG12	0.42	1.75	5	1
2:A:214:ASN:O	2:A:217:LYS:HG2	0.42	2.14	6	1
2:A:176:MET:O	2:A:206:LEU:HB2	0.42	2.14	9	1
2:A:142:ILE:HB	2:A:203:LEU:O	0.42	2.14	5	2
1:B:505:C:H4'	1:B:506:U:H5'	0.42	1.92	1	2
2:A:144:GLN:HG3	2:A:203:LEU:HB2	0.42	1.92	9	2
2:A:245:ARG:HH11	2:A:249:ARG:HB2	0.42	1.74	3	1
2:A:157:ILE:HG22	2:A:158:GLY:N	0.41	2.29	1	3
2:A:228:GLN:HB3	2:A:232:THR:CB	0.41	2.46	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:159:PRO:C	2:A:161:GLY:H	0.41	2.23	9	2
2:A:255:ARG:H	2:A:255:ARG:HG2	0.41	1.37	5	1
2:A:151:ASN:OD1	2:A:230:ILE:HG23	0.41	2.16	3	1
2:A:137:SER:HB3	2:A:208:THR:HG23	0.41	1.92	10	1
2:A:236:GLN:HB2	2:A:239:LEU:HB2	0.41	1.91	3	1
1:B:511:A:N6	2:A:183:VAL:HG22	0.41	2.30	8	1
1:B:502:A:C2'	2:A:255:ARG:HA	0.41	2.44	7	1
1:B:509:C:O2'	2:A:176:MET:HE2	0.41	2.15	1	1
1:B:502:A:N7	2:A:253:THR:HA	0.41	2.30	2	1
2:A:150:ILE:HG22	2:A:151:ASN:N	0.41	2.30	7	3
2:A:254:LEU:HD13	2:A:255:ARG:N	0.41	2.30	2	1
2:A:218:ALA:O	2:A:222:ILE:HG13	0.41	2.16	10	2
1:B:502:A:O2'	2:A:255:ARG:HD2	0.41	2.16	9	1
2:A:140:VAL:HG23	2:A:223:ARG:NE	0.41	2.30	3	1
2:A:147:TYR:HB2	2:A:152:PHE:HE2	0.41	1.76	8	1
2:A:149:GLU:HB3	2:A:203:LEU:CG	0.40	2.47	10	1
2:A:232:THR:OG1	2:A:236:GLN:HG3	0.40	2.17	2	1
2:A:224:ASN:O	2:A:228:GLN:HG3	0.40	2.16	3	1
2:A:151:ASN:HB2	2:A:155:LEU:CD2	0.40	2.46	5	1
2:A:150:ILE:CG2	2:A:151:ASN:H	0.40	2.28	2	1
2:A:164:LEU:HB3	2:A:175:ILE:HB	0.40	1.94	7	1
2:A:236:GLN:C	2:A:238:ASP:H	0.40	2.24	9	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	110/131 (84%)	80±2 (73±2%)	22±2 (20±2%)	7±1 (7±1%)	2	17
All	All	1100/1310 (84%)	803 (73%)	224 (20%)	73 (7%)	2	17

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	148	PRO	10
2	A	150	ILE	10
2	A	161	GLY	10
2	A	203	LEU	10
2	A	202	PRO	8
2	A	149	GLU	5
2	A	254	LEU	4
2	A	233	PRO	3
2	A	180	LYS	2
2	A	198	GLY	2
2	A	236	GLN	2
2	A	184	LYS	2
2	A	199	GLU	1
2	A	237	ASN	1
2	A	197	PRO	1
2	A	232	THR	1
2	A	181	GLY	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	99/112 (88%)	61±2 (61±2%)	38±2 (39±2%)	0 6
All	All	990/1120 (88%)	606 (61%)	384 (39%)	0 6

All 76 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	A	139	LYS	10
2	A	149	GLU	10
2	A	153	VAL	10
2	A	196	LEU	10
2	A	203	LEU	10
2	A	208	THR	10
2	A	219	VAL	10
2	A	226	LEU	10
2	A	230	ILE	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	A	244	LEU	10
2	A	247	LEU	10
2	A	253	THR	10
2	A	171	CYS	9
2	A	216	LYS	9
2	A	137	SER	8
2	A	249	ARG	8
2	A	147	TYR	8
2	A	232	THR	8
2	A	151	ASN	7
2	A	184	LYS	7
2	A	241	LYS	7
2	A	245	ARG	7
2	A	254	LEU	7
2	A	182	SER	7
2	A	165	LYS	7
2	A	250	LEU	7
2	A	169	LYS	6
2	A	180	LYS	6
2	A	243	GLN	6
2	A	211	THR	5
2	A	234	GLU	5
2	A	255	ARG	5
2	A	213	GLU	5
2	A	228	GLN	5
2	A	236	GLN	5
2	A	240	ARG	5
2	A	242	MET	5
2	A	141	MET	5
2	A	138	ASP	4
2	A	168	GLU	4
2	A	170	GLU	4
2	A	174	LYS	4
2	A	183	VAL	4
2	A	195	MET	4
2	A	144	GLN	3
2	A	146	GLU	3
2	A	235	ASP	3
2	A	238	ASP	3
2	A	156	LEU	3
2	A	200	ASP	3
2	A	239	LEU	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	A	162	ASN	3
2	A	172	ASN	3
2	A	227	LYS	3
2	A	201	GLU	3
2	A	155	LEU	3
2	A	166	ASN	3
2	A	251	ASN	3
2	A	164	LEU	3
2	A	140	VAL	2
2	A	237	ASN	2
2	A	221	GLN	2
2	A	175	ILE	2
2	A	178	ARG	2
2	A	199	GLU	2
2	A	135	ARG	2
2	A	246	GLU	2
2	A	145	ASP	2
2	A	231	GLU	1
2	A	176	MET	1
2	A	217	LYS	1
2	A	150	ILE	1
2	A	160	ARG	1
2	A	212	MET	1
2	A	206	LEU	1
2	A	134	THR	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	11/11 (100%)	7±0 (64±0%)	2±1 (23±9%)	0.44±0.00
All	All	104/110 (95%)	70 (67%)	25 (24%)	0.44

The overall RNA backbone suiteness is 0.10.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	502	A	10
1	B	503	U	10
1	B	504	A	10
1	B	506	U	10
1	B	507	A	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	508	A	10
1	B	511	A	10

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	507	A	10
1	B	505	C	7
1	B	501	U	4
1	B	502	A	2
1	B	503	U	2

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 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