WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2017 – 07:58 pm GMT

PDB ID : 1T2R
Title : Structural basis for 3' end recognition of nucleic acids by the Drosophila Argonaute 2 PAZ domain
Authors : Lingel, A.; Simon, B.; Izaurralde, E.; Sattler, M.
Deposited on : 2004-04-22

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:
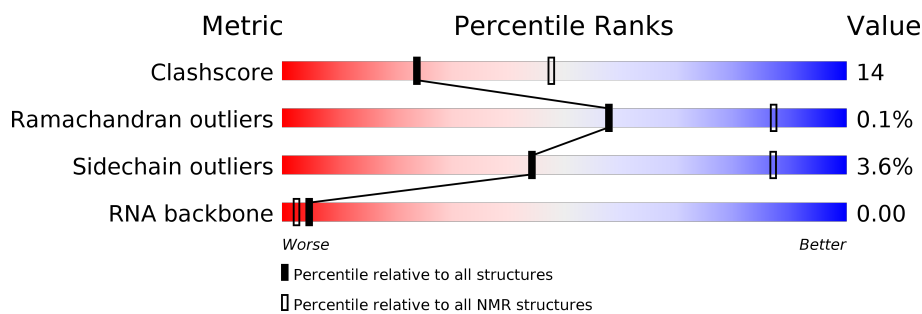
1   Overall quality at a glance   ⓘ

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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		0.1%
Sidechain outliers		3.6%
RNA backbone		0.00

Worse   Better

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367
RNA backbone	3398	623

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	5	20% 20% 60%
2	A	123	72% 22% 6%

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 1 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	A:4-A:119 (116)	0.42	1

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2029 atoms, of which 1007 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	2	65	19	23	8	13	2	0

- Molecule 2 is a protein called Argonaute 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	123	1964	626	984	170	179	5	0

There are 4 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q9VUQ5
A	2	ALA	-	CLONING ARTIFACT	UNP Q9VUQ5
A	3	MET	-	CLONING ARTIFACT	UNP Q9VUQ5
A	4	ALA	-	CLONING ARTIFACT	UNP Q9VUQ5

4 Residue-property plots ⓘ

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: 5'-R(*CP*UP*CP*AP*C)-3'

Chain B:

• Molecule 2: Argonaute 2
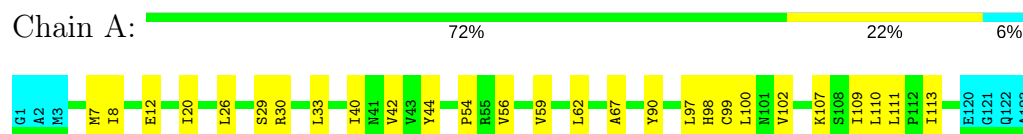
Chain A:

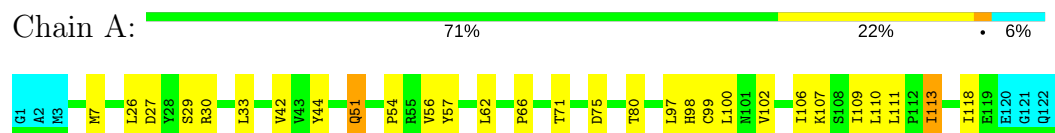## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'

Chain B:

• Molecule 2: Argonaute 2

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'

Chain B:

• Molecule 2: Argonaute 2

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'

Chain B:

• Molecule 2: Argonaute 2

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'
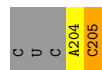
Chain B:

• Molecule 2: Argonaute 2
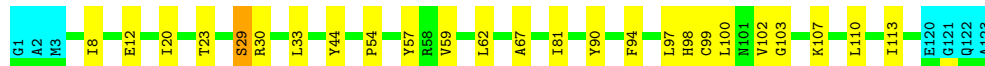
Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'
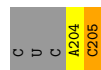
Chain B:

• Molecule 2: Argonaute 2
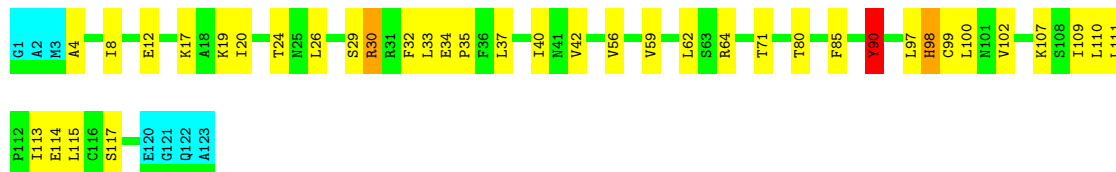
Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'
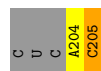
Chain B:

• Molecule 2: Argonaute 2

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'

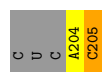Chain B:

• Molecule 2: Argonaute 2

Chain A:
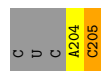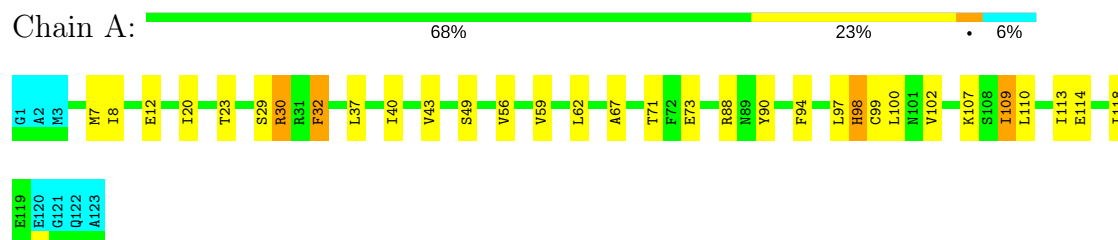
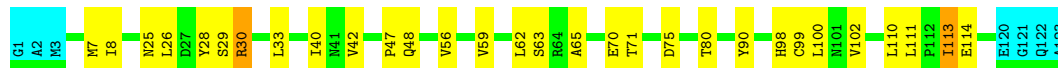### 4.2.8 Score per residue for model 8

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

Chain B:

- Molecule 2: Argonaute 2

Chain A:
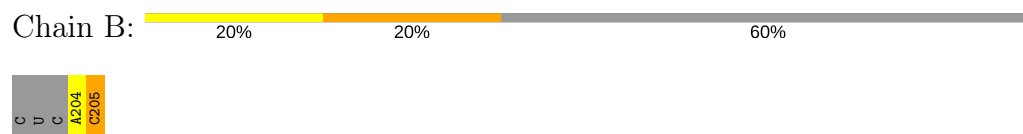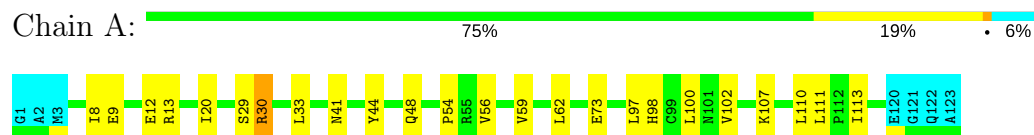
4.2.9 Score per residue for model 9

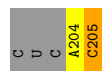- Molecule 1: 5'-R(*CP*UP*CP*AP*C)-3'

Chain B:

- Molecule 2: Argonaute 2

Chain A:
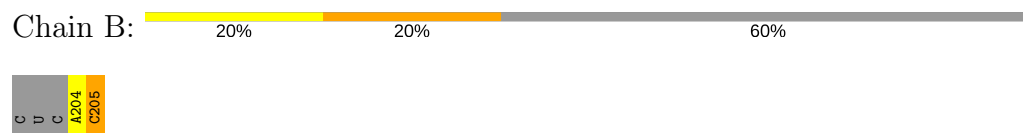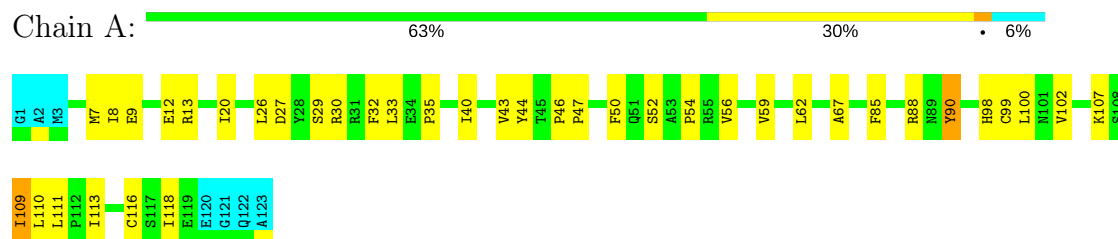
4.2.10 Score per residue for model 10

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

Chain B: 20%   20%   60%

C U C A204 C205

• Molecule 2: Argonaute 2

Chain A: 69%   24%   • 6%

G1 A2 M3 A4 M5 I8 E12 R13 K17 I20 N25 L26 S29 R30 L33 E34 P35 V42 V56 V59 L62 A67 Y90 L97 H98 C99 L100 N101 V102 K107 S108 I109 L110 I113 C116 E119 E120 G121 Q122 A123
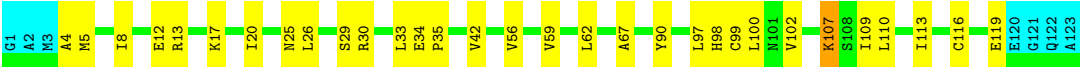
5 Refinement protocol and experimental data overview ⓘ

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

Of the 150 calculated structures, 10 were deposited, based on the following criterion: *lowest energies.*

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

Software name	Classification	Version
ARIA1.2, CNS1.1	refinement	
NMRVIEW	structure solution	
ARIA/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 ⓘ

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	B	0.21±0.02	0±0/46 (0.0±0.0%)	0.83±0.13	0±0/69 (0.0±0.0%)
2	A	0.43±0.12	1±1/960 (0.1±0.1%)	0.44±0.03	0±1/1302 (0.0±0.0%)
All	All	0.44	5/10060 (0.0%)	0.47	2/13710 (0.0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	90	TYR	CE2-CZ	-14.04	1.20	1.38	5	2
2	A	90	TYR	CE1-CZ	13.46	1.56	1.38	5	2
2	A	32	PHE	CE1-CZ	5.65	1.48	1.37	5	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	90	TYR	CE1-CZ-OH	-5.13	106.23	120.10	5	1
2	A	90	TYR	CZ-CE2-CD2	5.00	124.30	119.80	5	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	42	23	23	5±1
2	A	935	943	943	22±5
All	All	9770	9660	9660	266

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:A:107:LYS:HD2	2:A:109:ILE:HG23	0.87	1.45	9	3
2:A:30:ARG:HG2	2:A:98:HIS:HB2	0.86	1.48	5	8
2:A:30:ARG:HG3	2:A:62:LEU:HD13	0.81	1.50	7	8
2:A:57:TYR:HB3	2:A:102:VAL:HG21	0.79	1.55	4	1
2:A:12:GLU:OE2	2:A:19:LYS:HA	0.79	1.78	5	1
1:B:204:A:OP2	2:A:107:LYS:HE3	0.74	1.82	9	3
2:A:65:ALA:HB3	2:A:70:GLU:HG3	0.73	1.60	3	1
2:A:27:ASP:HA	2:A:30:ARG:HG2	0.73	1.59	2	1
1:B:204:A:H2'	1:B:204:A:N3	0.73	1.97	7	5
1:B:204:A:N3	1:B:204:A:H2'	0.72	1.98	10	5
2:A:26:LEU:HD22	2:A:97:LEU:HD22	0.66	1.68	1	1
2:A:30:ARG:HE	2:A:62:LEU:HD13	0.65	1.51	9	1
2:A:29:SER:O	2:A:33:LEU:HG	0.65	1.91	4	8
2:A:26:LEU:HG	2:A:30:ARG:HB2	0.65	1.68	1	1
2:A:102:VAL:HG23	2:A:109:ILE:HG13	0.64	1.70	6	6
2:A:30:ARG:HD2	2:A:98:HIS:HB2	0.64	1.68	2	1
2:A:106:ILE:HD13	2:A:106:ILE:H	0.62	1.54	2	1
2:A:90:TYR:OH	2:A:115:LEU:HD12	0.62	1.94	5	1
2:A:51:GLN:HE21	2:A:51:GLN:HA	0.62	1.53	1	1
2:A:59:VAL:HG22	2:A:102:VAL:HG12	0.61	1.70	3	5
2:A:59:VAL:HG11	2:A:100:LEU:HD23	0.61	1.73	7	3
2:A:8:ILE:CG1	2:A:114:GLU:HA	0.60	2.26	5	1
2:A:12:GLU:HG2	2:A:20:ILE:H	0.60	1.55	10	1
1:B:204:A:H4'	1:B:205:C:O4'	0.60	1.95	10	2
1:B:204:A:H5'	1:B:205:C:O4'	0.60	1.95	1	8
2:A:44:TYR:O	2:A:54:PRO:HA	0.59	1.97	9	5
2:A:59:VAL:HA	2:A:102:VAL:HG23	0.58	1.74	4	1
2:A:100:LEU:HD11	2:A:113:ILE:HB	0.56	1.76	7	1
2:A:59:VAL:HA	2:A:102:VAL:HG12	0.56	1.77	10	3
2:A:7:MET:O	2:A:11:LEU:HG	0.56	2.01	6	1
1:B:204:A:O5'	1:B:205:C:C1'	0.56	2.54	10	2
2:A:85:PHE:O	2:A:90:TYR:HB3	0.56	2.01	5	1
2:A:100:LEU:HD12	2:A:111:LEU:O	0.55	2.02	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:204:A:O5'	1:B:205:C:C6	0.55	2.59	3	5
2:A:43:VAL:HG22	2:A:56:VAL:HG22	0.55	1.78	9	2
2:A:29:SER:HA	2:A:32:PHE:HD2	0.54	1.62	7	1
2:A:37:LEU:CD1	2:A:62:LEU:HD11	0.54	2.32	7	1
2:A:100:LEU:O	2:A:110:LEU:HA	0.54	2.02	1	7
2:A:67:ALA:HB2	2:A:99:CYS:SG	0.54	2.43	6	5
2:A:102:VAL:CG2	2:A:111:LEU:HG	0.53	2.33	1	6
2:A:102:VAL:HG21	2:A:111:LEU:HG	0.53	1.80	1	4
2:A:71:THR:HG22	2:A:80:THR:HG22	0.53	1.80	1	2
2:A:26:LEU:HB2	2:A:97:LEU:HA	0.52	1.82	5	1
2:A:30:ARG:HH21	2:A:62:LEU:HD22	0.52	1.65	9	1
2:A:27:ASP:HB2	2:A:98:HIS:CE1	0.52	2.39	1	3
2:A:41:ASN:OD1	2:A:56:VAL:HG13	0.51	2.04	8	1
2:A:12:GLU:HG2	2:A:20:ILE:HG12	0.51	1.82	6	6
2:A:42:VAL:HG21	2:A:116:CYS:HB3	0.51	1.80	10	1
1:B:204:A:C2	2:A:107:LYS:NZ	0.51	2.73	10	1
2:A:47:PRO:HB3	2:A:90:TYR:CD2	0.51	2.41	6	1
2:A:107:LYS:HD2	2:A:109:ILE:CG2	0.51	2.29	5	1
2:A:5:MET:HE1	2:A:13:ARG:HD3	0.50	1.83	10	1
2:A:7:MET:SD	2:A:118:ILE:HB	0.50	2.46	9	3
2:A:8:ILE:O	2:A:12:GLU:HG3	0.50	2.07	6	7
1:B:204:A:OP2	2:A:107:LYS:HE2	0.50	2.07	6	1
1:B:204:A:N3	1:B:204:A:C2'	0.50	2.75	4	5
2:A:30:ARG:CZ	2:A:113:ILE:HD12	0.49	2.36	6	3
2:A:102:VAL:HG22	2:A:103:GLY:H	0.49	1.67	4	1
2:A:47:PRO:HB3	2:A:90:TYR:CE2	0.49	2.42	3	1
2:A:107:LYS:HG2	2:A:109:ILE:HG23	0.49	1.82	10	1
1:B:204:A:O5'	1:B:205:C:H1'	0.49	2.07	10	1
2:A:97:LEU:HD13	2:A:113:ILE:HG22	0.49	1.83	7	1
2:A:40:ILE:CG1	2:A:59:VAL:HB	0.48	2.38	9	4
2:A:94:PHE:O	2:A:97:LEU:HG	0.48	2.08	7	2
2:A:71:THR:HA	2:A:80:THR:HA	0.48	1.84	5	1
1:B:204:A:C2'	1:B:204:A:N3	0.48	2.76	6	5
2:A:66:PRO:HG3	2:A:98:HIS:CE1	0.48	2.43	1	1
2:A:88:ARG:HA	2:A:88:ARG:HE	0.48	1.68	7	1
2:A:12:GLU:OE2	2:A:19:LYS:HD2	0.48	2.08	5	1
2:A:64:ARG:N	2:A:64:ARG:HD2	0.48	2.24	5	1
2:A:42:VAL:O	2:A:56:VAL:HA	0.48	2.08	1	6
1:B:204:A:C5'	1:B:205:C:O4'	0.48	2.61	4	3
2:A:88:ARG:HA	2:A:88:ARG:NE	0.47	2.23	7	1
2:A:8:ILE:HG12	2:A:114:GLU:HA	0.47	1.87	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:26:LEU:H	2:A:26:LEU:HD12	0.47	1.70	2	3
1:B:205:C:O3'	2:A:109:ILE:HB	0.46	2.11	10	1
2:A:99:CYS:HB3	2:A:110:LEU:HB3	0.46	1.87	2	2
2:A:97:LEU:HD12	2:A:97:LEU:O	0.46	2.11	6	1
2:A:4:ALA:HB1	2:A:117:SER:OG	0.46	2.11	5	1
2:A:46:PRO:HG2	2:A:52:SER:HB3	0.46	1.85	9	1
2:A:26:LEU:HB2	2:A:30:ARG:HD3	0.45	1.87	2	1
2:A:44:TYR:OH	2:A:112:PRO:HD2	0.45	2.11	2	1
2:A:16:LEU:HD11	2:A:26:LEU:HA	0.45	1.88	2	1
2:A:26:LEU:HD22	2:A:97:LEU:HB2	0.45	1.88	10	1
2:A:58:ARG:C	2:A:58:ARG:HD2	0.45	2.32	2	1
1:B:204:A:C2	2:A:57:TYR:CE1	0.45	3.05	1	1
2:A:102:VAL:HG13	2:A:103:GLY:N	0.45	2.27	4	1
2:A:22:ASN:ND2	2:A:23:THR:HG23	0.45	2.27	2	1
2:A:7:MET:HB3	2:A:113:ILE:CG1	0.44	2.43	1	3
1:B:204:A:OP1	1:B:205:C:H1'	0.44	2.11	6	1
2:A:40:ILE:HG13	2:A:59:VAL:HB	0.44	1.87	6	2
2:A:99:CYS:CB	2:A:110:LEU:HB3	0.44	2.42	5	2
2:A:29:SER:HA	2:A:32:PHE:CD2	0.44	2.46	7	1
2:A:30:ARG:HA	2:A:33:LEU:HB2	0.44	1.88	9	1
2:A:63:SER:HB2	2:A:70:GLU:OE2	0.44	2.12	3	1
2:A:34:GLU:N	2:A:35:PRO:HD2	0.44	2.28	5	3
2:A:30:ARG:NH1	2:A:97:LEU:HA	0.43	2.28	2	1
1:B:205:C:OP1	2:A:111:LEU:HD22	0.43	2.13	2	1
2:A:4:ALA:HA	2:A:119:GLU:HG2	0.43	1.90	10	1
2:A:30:ARG:NH1	2:A:113:ILE:HD12	0.43	2.28	8	3
2:A:107:LYS:O	2:A:107:LYS:HG2	0.43	2.13	10	1
2:A:33:LEU:O	2:A:37:LEU:HD23	0.43	2.14	5	2
2:A:37:LEU:O	2:A:40:ILE:HG12	0.43	2.14	7	1
2:A:13:ARG:O	2:A:17:LYS:HD2	0.43	2.14	10	1
2:A:67:ALA:HB1	2:A:81:ILE:HB	0.42	1.91	4	1
2:A:85:PHE:HB3	2:A:90:TYR:CD2	0.42	2.49	9	1
2:A:9:GLU:O	2:A:13:ARG:HG3	0.42	2.14	8	2
1:B:204:A:C6	2:A:107:LYS:HG2	0.42	2.50	7	1
2:A:59:VAL:HG22	2:A:102:VAL:CG1	0.42	2.45	10	1
2:A:59:VAL:HG11	2:A:100:LEU:HD11	0.42	1.90	2	1
2:A:30:ARG:NE	2:A:30:ARG:HA	0.42	2.29	5	1
2:A:107:LYS:HD3	2:A:107:LYS:C	0.42	2.34	7	1
1:B:204:A:P	2:A:107:LYS:HE3	0.42	2.55	9	1
2:A:12:GLU:CD	2:A:20:ILE:H	0.41	2.18	5	1
2:A:12:GLU:OE1	2:A:20:ILE:HG12	0.41	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:A:97:LEU:O	2:A:97:LEU:HD12	0.41	2.14	8	1
2:A:44:TYR:O	2:A:46:PRO:HD3	0.41	2.14	2	1
2:A:25:ASN:HB2	2:A:28:TYR:CE2	0.41	2.51	3	1
2:A:110:LEU:HD12	2:A:110:LEU:N	0.41	2.31	6	1
2:A:110:LEU:HD22	2:A:110:LEU:N	0.41	2.31	3	1
2:A:25:ASN:C	2:A:27:ASP:H	0.41	2.18	2	1
2:A:99:CYS:HB2	2:A:110:LEU:HB3	0.41	1.93	10	3
2:A:100:LEU:HD11	2:A:116:CYS:SG	0.41	2.56	9	1
2:A:37:LEU:HD13	2:A:62:LEU:HD11	0.41	1.92	7	1
2:A:32:PHE:O	2:A:35:PRO:HD2	0.41	2.16	9	1
2:A:44:TYR:CE1	2:A:111:LEU:HB3	0.41	2.51	9	1
2:A:47:PRO:HG2	2:A:50:PHE:CD1	0.41	2.51	9	1
2:A:50:PHE:CE1	2:A:88:ARG:HG3	0.41	2.51	6	1
2:A:106:ILE:HG13	2:A:107:LYS:N	0.41	2.31	1	1
2:A:113:ILE:HA	2:A:116:CYS:SG	0.40	2.56	9	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	A	116/123 (94%)	112±1 (97±1%)	4±1 (3±1%)	0±0 (0±0%)	58	87
All	All	1160/1230 (94%)	1120 (97%)	39 (3%)	1 (0%)	58	87

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	A	98	HIS	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	A	106/109 (97%)	102±2 (96±2%)	4±2 (4±2%)	44	87
All	All	1060/1090 (97%)	1022 (96%)	38 (4%)	44	87

All 21 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	90	TYR	5
2	A	30	ARG	4
2	A	113	ILE	2
2	A	109	ILE	2
2	A	75	ASP	2
2	A	23	THR	2
2	A	25	ASN	2
2	A	48	GLN	2
2	A	29	SER	2
2	A	98	HIS	2
2	A	107	LYS	2
2	A	73	GLU	2
2	A	71	THR	1
2	A	58	ARG	1
2	A	51	GLN	1
2	A	88	ARG	1
2	A	49	SER	1
2	A	17	LYS	1
2	A	24	THR	1
2	A	106	ILE	1
2	A	32	PHE	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	1/5 (20%)	1±0 (100±0%)	0±0 (0±0%)	0.00±0.00
All	All	10/50 (20%)	10 (100%)	0 (0%)	0.00

The overall RNA backbone suiteness is 0.00.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	205	C	10

There are no RNA pucker outliers to report.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided