Full wwPDB NMR Structure Validation Report (i)

Oct 17, 2021 – 09:48 AM EDT

PDB ID	:	1KQQ
Title	:	Solution Structure of the Dead ringer ARID-DNA Complex
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Deposited on	:	2002-01-07

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 (i) symbol.

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

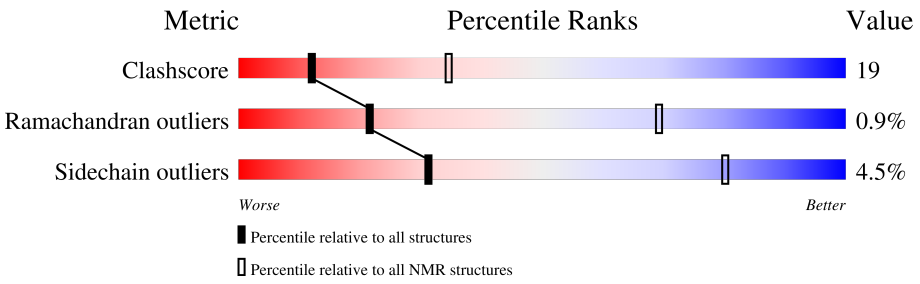
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	15	60% 33% 7%
2	C	15	73% 20% 7%
3	A	139	53% 34% • 6% 6%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 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:9-A:130 (122)	0.19	18

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3120 atoms, of which 1435 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	15	480	148	173	53	92	14	0

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	C	15	471	145	169	59	84	14	0

- Molecule 3 is a protein called DEAD RINGER PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	A	131	2169	692	1093	183	197	4	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q24573
A	2	SER	-	cloning artifact	UNP Q24573
A	96	LEU	PHE	engineered mutation	UNP Q24573

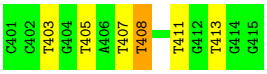
4 Residue-property plots (i)

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: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 33% 7%

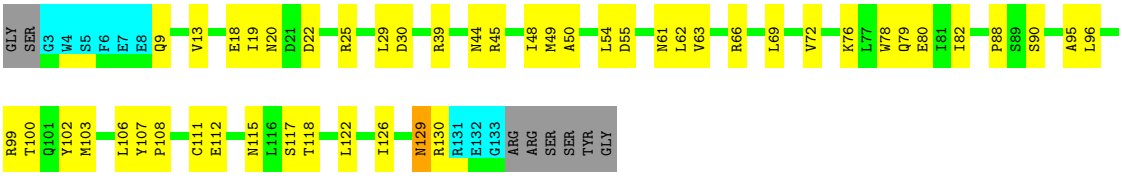


• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 73% 20% 7%

• Molecule 3: DEAD RINGER PROTEIN

Chain A: 53% 34% 6% 6%



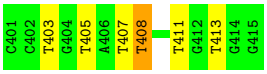
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

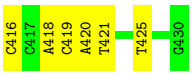
• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 33% 7%



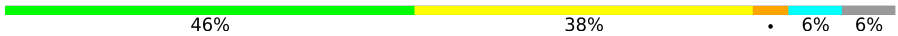
• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C:



• Molecule 3: DEAD RINGER PROTEIN

Chain A:



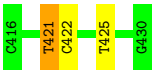
4.2.2 Score per residue for model 2

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B:

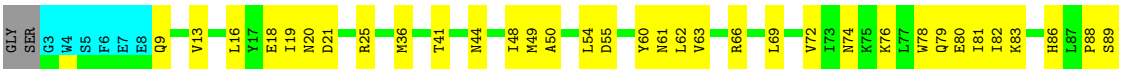
• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C:



• Molecule 3: DEAD RINGER PROTEIN

Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 40% 53% 7%

C401 C402 T403 G404 T405 A406 T407 T408 G409 A410 T411 G412 T413 G414 G415

• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 60% 33% 7%

C416 A420 T421 C422 A423 A424 T425 G430

• Molecule 3: DEAD RINGER PROTEIN

Chain A: 56% 29% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 Q9 V13 E18 I19 D22 R25 L29 F33 I43 N44 I48 M49 A50 L54 L62 V63 R66 V72 I73 N74 K75 K76 L77 W78 Q79 E80 I81 I82 P88 S89 S90 A95 R99 Y102 M103 K104

Y105 L106 Y107 P108 C111 E112 N115 L116 S117 T118 A125 I126 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

4.2.4 Score per residue for model 4

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 33% 7%

C401 C402 T403 G404 T405 A406 T407 T408 T411 G412 T413 G414 G415

• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 73% 27%

C416 A420 T421 T425 G430

• Molecule 3: DEAD RINGER PROTEIN

Chain A: 54% 32% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 E18 I19 N20 D21 D22 P23 K24 R25 K38 R39 R45 I48 M49 A50 L62 V63 R66 V72 I73 N74 K75 K76 L77 W78 Q79 E80 I81 I82 L85 P88 S89 S90 A95 L96 T97 L98 R99 Y102 M103 L106

Y107 P108 C111 E112 N115 L116 S117 T118 P119 A120 E121 L122 I126 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 53% 40% 7%

C401 C402 T403 G404 T405 A406 T407 T408 G409 A410 T411 G412 T413 G414 G415

- Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 60% 33% 7%

C416 C419 A420 T421 C422 A423 A424 T425 G430

- Molecule 3: DEAD RINGER PROTEIN

Chain A: 53% 32% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 Q9 F10 K11 Q12 V13 L16 Y17 E18 I19 N20 R25 K26 L29 D30 F33 I43 N44 R45 I48 M49 A50 L54 D55 L59 Y60 V63 I64 A65 R66 L69 V72 K76 L77 W78 Q79 E80 I81 I82 P88

S89 S90 A95 L96 T97 L98 R99 T100 Q101 Y102 M103 L106 Y107 P108 E112 L116 L122 I126 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

4.2.6 Score per residue for model 6

- Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 33% 7%

C401 C402 T403 G404 T405 A406 T407 T408 T411 G412 T413 G414 G415

- Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

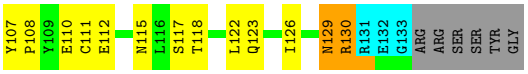
Chain C: 73% 20% 7%

C416 C419 A420 T421 T425 G430

- Molecule 3: DEAD RINGER PROTEIN

Chain A: 56% 28% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 Q9 F10 K11 Q12 V13 E18 I19 R25 L29 F33 N44 I48 M49 A50 L54 D55 V63 R66 L69 V72 K76 L77 W78 Q79 E80 I81 I82 P88 S89 S90 L96 R99 T100 Q101 Y102 M103



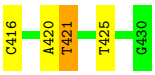
4.2.7 Score per residue for model 7

- Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B:

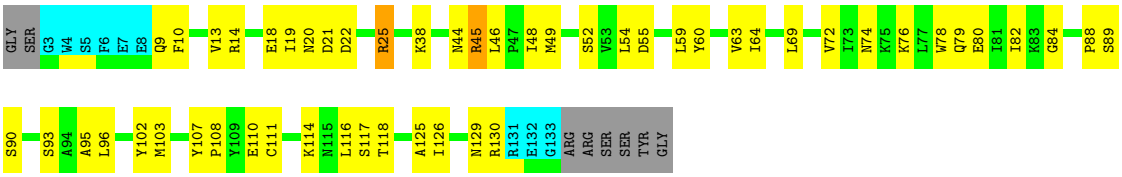
- Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C:



- Molecule 3: DEAD RINGER PROTEIN

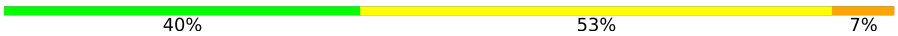
Chain A:

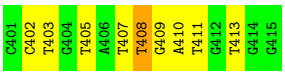


4.2.8 Score per residue for model 8

- Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

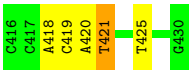
Chain B:





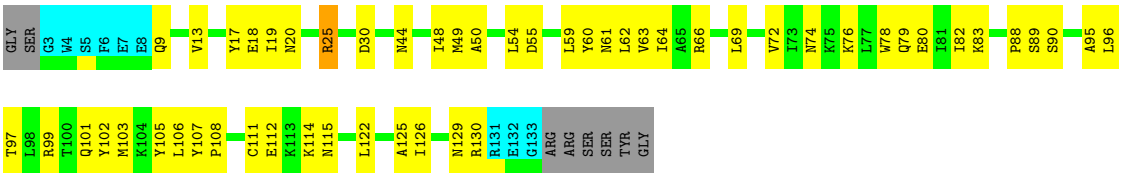
- Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C:



- Molecule 3: DEAD RINGER PROTEIN

Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

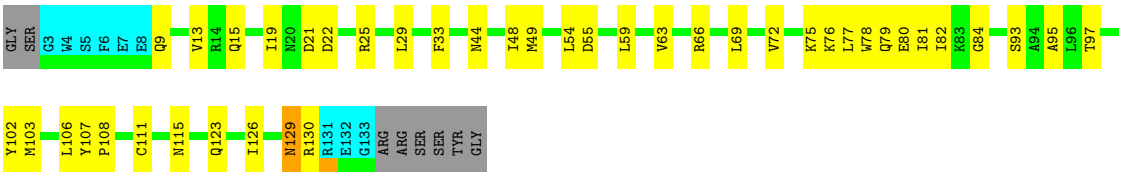
Chain B: 53% 40% 7%

- Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 67% 27% 7%

- Molecule 3: DEAD RINGER PROTEIN

Chain A: 58% 29% • 6% 6%



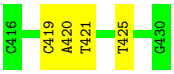
4.2.10 Score per residue for model 10

- Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 27% 13%

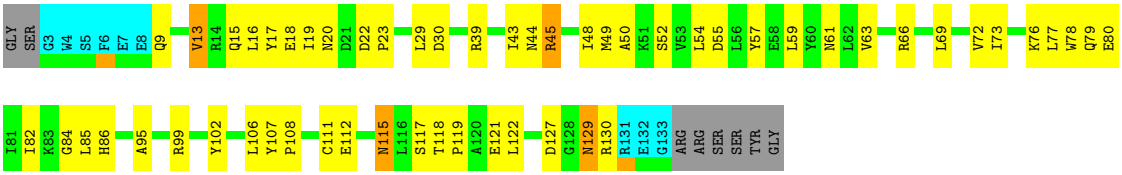
- Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 73% 27%



• Molecule 3: DEAD RINGER PROTEIN

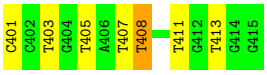
Chain A: 47% 37% • 6% 6%



4.2.11 Score per residue for model 11

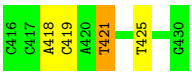
• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 53% 40% 7%



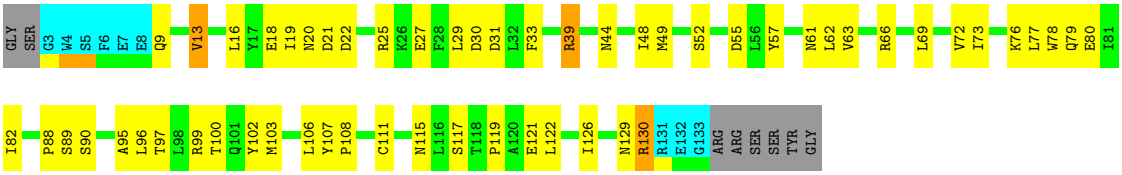
• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 73% 20% 7%



• Molecule 3: DEAD RINGER PROTEIN

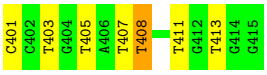
Chain A: 47% 38% • 6% 6%



4.2.12 Score per residue for model 12

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 53% 40% 7%

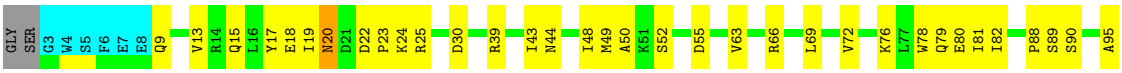


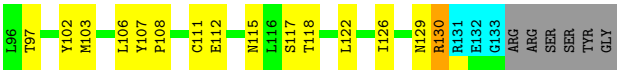
• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 87% 7% 7%

• Molecule 3: DEAD RINGER PROTEIN

Chain A:

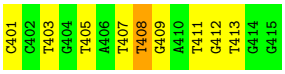




4.2.13 Score per residue for model 13

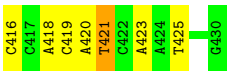
• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B:



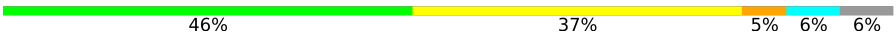
• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

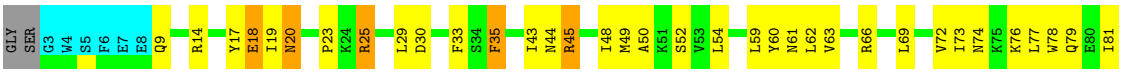
Chain C:



• Molecule 3: DEAD RINGER PROTEIN

Chain A:





4.2.14 Score per residue for model 14

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B:

• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 60% 33% 7%

C416 C417 A418 C419 A420 T421 C422 T425 G430

• Molecule 3: DEAD RINGER PROTEIN

Chain A: 44% 40% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 Q9 V13 R14 Q15 L16 Y17 E18 I19 N20 D21 D22 P23 K24 R25 L29 D30 D31 L32 M36 Q37 K38 R39 G40 T41 N44 R45 I48 M49 A50 L54 D55 L56 L59 Y60 N61 L62 V63 R66 V72 K76 L77 W78

Q79 E80 I81 I82 P88 S89 S90 A94 A95 L96 T100 Q101 Y102 M103 K104 Y105 L106 Y107 P108 C111 E112 N115 L116 S117 T118 P119 A120 E121 L122 I126 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

4.2.15 Score per residue for model 15

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 33% 7%

C401 C402 T403 G404 T405 A406 T407 T408 T411 G412 T413 G414 G415

• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 73% 20% 7%

C416 A420 T421 T425 G430

• Molecule 3: DEAD RINGER PROTEIN

Chain A: 54% 30% • 6% 6%

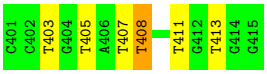
GLY SER G3 W4 S5 F6 E7 E8 Q9 F10 V13 R14 Q15 L16 N20 R25 L32 F35 M36 R39 N44 R45 L46 F47 I48 M49 A50 L54 Y57 N61 L62 V63 R66 L69 V72 I73 K76 L77 W78 Q79 E80 L96 R99 T100

Q101 Y102 M103 K104 Y105 L106 Y107 P108 Y109 E110 C111 E112 S117 T118 E121 L122 I126 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

4.2.16 Score per residue for model 16

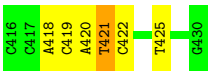
• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 33% 7%



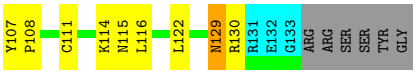
• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C:



• Molecule 3: DEAD RINGER PROTEIN

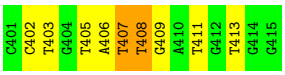
Chain A:



4.2.17 Score per residue for model 17

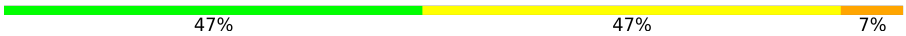
• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

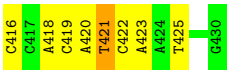
Chain B:



• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

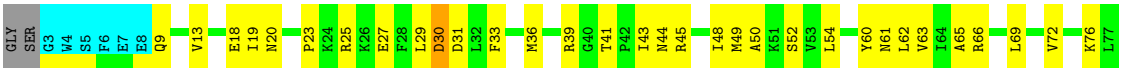
Chain C:





• Molecule 3: DEAD RINGER PROTEIN

Chain A:



4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 60% 27% 13%

C401 C402 T403 G404 T405 A406 T407 T408 T411 G412 T413 G414 G415

• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 80% 13% 7%

C416 A420 T421 T425 G430

• Molecule 3: DEAD RINGER PROTEIN

Chain A: 47% 38% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 Q9 V13 R14 Q15 E18 I19 N20 R25 L29 M36 T41 N44 R45 I48 M49 A50 L54 Y57 Y60 N61 L62 V63 I64 A65 R66 L69 V72 I73 K76 L77 W78 Q79 E80 I81 I82 P88 S89

S90 A95 L96 R99 Y102 M103 K104 Y105 L106 Y107 P108 Y109 E110 C111 E112 N115 L116 S117 T118 L122 Q123 A124 A125 I126 D127 G128 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

4.2.19 Score per residue for model 19

• Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 53% 40% 7%

C401 C402 T403 G404 T405 A406 T407 T408 T411 G412 T413 G414 G415

• Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 67% 27% 7%

C416 A420 T421 C422 T425 G430

• Molecule 3: DEAD RINGER PROTEIN

Chain A: 50% 35% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 Q9 V13 Y17 E18 I19 N20 D21 D22 P23 K24 R25 K26 E27 F28 L29 D30 F33 R39 I43 N44 R45 I48 M49 S52 D55 L56 Y57 Y60 N61 L62 V63 I64 A65 R66 L69 V72 K76 L77 W78 Q79

E80 I81 I82 K83 G84 T97 L98 R99 Y102 M103 L106 Y107 P108 Y109 E110 K114 N115 L116 S117 T118 L122 I126 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

4.2.20 Score per residue for model 20

- Molecule 1: 5'-D(*CP*CP*TP*GP*TP*AP*TP*TP*GP*AP*TP*GP*TP*GP*G)-3'

Chain B: 53% 40% 7%

C401 C402 T403 G404 T405 A406 T407 T408 T411 G412 T413 G414 G415

- Molecule 2: 5'-D(*CP*CP*AP*CP*AP*TP*CP*AP*AP*TP*AP*CP*AP*GP*G)-3'

Chain C: 60% 33% 7%

C416 C417 A418 C419 A420 T421 C422 T425 G430

- Molecule 3: DEAD RINGER PROTEIN

Chain A: 53% 33% • 6% 6%

GLY SER G3 W4 S5 F6 E7 E8 Q9 V13 R14 Q15 L16 Y17 E18 I19 N20 K24 R25 L29 D30 N44 I48 M49 A50 L54 Y57 E58 L59 Y60 N61 L62 V63 R66 L69 V72 K76 L77 W78 Q79 E80 I81 I82 K83 G84 P88 S89 S90

L96 T97 L98 R99 Y102 L106 Y107 P108 C111 E112 N115 L116 S117 T118 I126 N129 R130 R131 E132 G133 ARG ARG SER SER TYR GLY

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

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	B	1.12±0.01	4±1/343 (1.3± 0.3%)	1.64±0.01	11±1/529 (2.0± 0.1%)
2	C	0.99±0.02	1±0/339 (0.2± 0.1%)	1.57±0.01	4±0/520 (0.8± 0.0%)
3	A	1.01±0.00	0±0/1019 (0.0± 0.0%)	0.92±0.00	0±0/1376 (0.0± 0.0%)
All	All	1.03	103/34020 (0.3%)	1.26	296/48500 (0.6%)

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
1	B	408	DT	C5-C7	5.75	1.53	1.50	3	18
2	C	425	DT	C5-C7	5.55	1.53	1.50	5	13
1	B	411	DT	C5-C7	5.49	1.53	1.50	16	18
1	B	405	DT	C5-C7	5.49	1.53	1.50	6	19
1	B	413	DT	C5-C7	5.43	1.53	1.50	20	14
1	B	407	DT	C5-C7	5.31	1.53	1.50	10	7
1	B	403	DT	C5-C7	5.28	1.53	1.50	3	14

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	421	DT	C6-C5-C7	-6.49	119.00	122.90	17	20
1	B	407	DT	C6-C5-C7	-6.17	119.20	122.90	9	20
1	B	408	DT	C6-C5-C7	-6.10	119.24	122.90	16	20
2	C	421	DT	C4-C5-C6	6.06	121.64	118.00	11	20
2	C	425	DT	C6-C5-C7	-5.90	119.36	122.90	3	20
1	B	413	DT	C6-C5-C7	-5.84	119.40	122.90	9	20
1	B	405	DT	C6-C5-C7	-5.74	119.46	122.90	2	20
1	B	411	DT	C6-C5-C7	-5.58	119.55	122.90	8	20
1	B	403	DT	C6-C5-C7	-5.57	119.56	122.90	12	18
2	C	425	DT	C4-C5-C6	5.45	121.27	118.00	8	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	407	DT	C4-C5-C6	5.36	121.22	118.00	14	20
1	B	408	DT	C4-C5-C6	5.36	121.22	118.00	7	18
1	B	405	DT	C4-C5-C6	5.29	121.17	118.00	10	19
1	B	413	DT	C4-C5-C6	5.29	121.17	118.00	17	18
1	B	411	DT	C4-C5-C6	5.26	121.15	118.00	4	14
1	B	403	DT	C4-C5-C6	5.25	121.15	118.00	10	9

There are no chirality outliers.

There are no planarity outliers.

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	B	307	173	173	5±2
2	C	302	169	169	5±2
3	A	999	1032	1032	54±8
All	All	32160	27480	27480	1154

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:103:MET:SD	3:A:122:LEU:HD21	0.92	2.05	12	2
2:C:416:DC:H6	2:C:416:DC:HO5'	0.92	0.93	1	6
1:B:401:DC:HO5'	1:B:401:DC:H6	0.89	0.90	13	3
3:A:60:TYR:CE1	3:A:64:ILE:HD11	0.87	2.05	5	1
3:A:9:GLN:O	3:A:13:VAL:HG12	0.85	1.71	9	10
3:A:63:VAL:HG21	3:A:102:TYR:CE2	0.81	2.10	20	20
3:A:49:MET:SD	3:A:54:LEU:HD13	0.74	2.23	8	12
3:A:49:MET:SD	3:A:97:THR:HG21	0.74	2.23	4	7
2:C:416:DC:HO5'	2:C:416:DC:H6	0.74	1.22	19	3
3:A:99:ARG:NH1	3:A:129:ASN:ND2	0.72	2.37	8	4
3:A:20:ASN:HD21	3:A:25:ARG:NH1	0.71	1.84	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:106:LEU:HD12	3:A:106:LEU:N	0.70	2.02	14	16
2:C:416:DC:H6	2:C:416:DC:O5'	0.70	1.70	3	9
1:B:401:DC:H6	1:B:401:DC:O5'	0.70	1.66	11	3
3:A:129:ASN:ND2	3:A:130:ARG:N	0.70	2.40	9	11
3:A:20:ASN:HD21	3:A:25:ARG:HH11	0.69	1.30	15	1
3:A:99:ARG:NH1	3:A:129:ASN:HD21	0.69	1.85	2	4
3:A:9:GLN:O	3:A:13:VAL:HG13	0.69	1.88	8	6
3:A:126:ILE:CG2	3:A:130:ARG:NH2	0.68	2.56	8	1
3:A:127:ASP:OD1	3:A:128:GLY:N	0.68	2.27	18	1
3:A:103:MET:SD	3:A:126:ILE:HD11	0.67	2.29	14	9
3:A:62:LEU:HD22	3:A:66:ARG:HH22	0.66	1.49	16	2
3:A:129:ASN:OD1	3:A:130:ARG:N	0.66	2.28	8	9
3:A:107:TYR:N	3:A:108:PRO:CD	0.66	2.59	13	20
3:A:10:PHE:CZ	3:A:14:ARG:NE	0.65	2.64	7	1
3:A:107:TYR:CZ	3:A:111:CYS:SG	0.64	2.88	11	4
3:A:10:PHE:CE1	3:A:14:ARG:NE	0.64	2.65	15	1
3:A:61:ASN:H	3:A:61:ASN:HD22	0.64	1.35	19	1
3:A:72:VAL:O	3:A:76:LYS:N	0.64	2.30	16	20
3:A:69:LEU:HD13	3:A:102:TYR:CD1	0.63	2.28	16	5
3:A:45:ARG:O	3:A:45:ARG:NE	0.63	2.32	18	1
3:A:99:ARG:NH1	3:A:129:ASN:OD1	0.62	2.32	6	7
3:A:107:TYR:CE1	3:A:111:CYS:SG	0.62	2.93	11	6
3:A:103:MET:CE	3:A:126:ILE:HD11	0.62	2.25	9	2
3:A:129:ASN:C	3:A:129:ASN:HD22	0.62	1.98	10	11
3:A:10:PHE:CE2	3:A:14:ARG:NH2	0.62	2.67	7	1
3:A:103:MET:SD	3:A:122:LEU:CD2	0.61	2.89	17	2
2:C:416:DC:O5'	2:C:416:DC:C6	0.61	2.52	15	9
3:A:62:LEU:O	3:A:66:ARG:NH1	0.61	2.34	18	9
1:B:408:DT:P	3:A:48:ILE:O	0.61	2.59	12	20
3:A:9:GLN:NE2	3:A:43:ILE:O	0.61	2.34	5	3
3:A:44:ASN:O	3:A:45:ARG:NE	0.61	2.34	1	1
3:A:49:MET:O	3:A:50:ALA:HB3	0.61	1.95	14	16
3:A:20:ASN:ND2	3:A:20:ASN:O	0.60	2.34	15	2
3:A:19:ILE:HD13	3:A:25:ARG:NH2	0.60	2.12	1	9
3:A:25:ARG:HH11	3:A:25:ARG:CG	0.60	2.09	4	4
3:A:9:GLN:NE2	3:A:44:ASN:O	0.60	2.34	15	15
2:C:421:DT:C4	2:C:422:DC:N4	0.60	2.70	2	8
3:A:129:ASN:ND2	3:A:129:ASN:C	0.60	2.55	5	11
3:A:30:ASP:OD1	3:A:31:ASP:N	0.60	2.35	17	2
3:A:107:TYR:OH	3:A:119:PRO:N	0.60	2.35	10	5
3:A:117:SER:OG	3:A:118:THR:N	0.60	2.33	13	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:35:PHE:CZ	3:A:112:GLU:OE1	0.60	2.55	13	2
3:A:63:VAL:HG11	3:A:102:TYR:CZ	0.60	2.31	20	4
3:A:97:THR:O	3:A:101:GLN:NE2	0.59	2.35	8	1
3:A:57:TYR:CZ	3:A:61:ASN:OD1	0.59	2.55	18	2
3:A:74:ASN:OD1	3:A:125:ALA:HB1	0.59	1.97	3	5
3:A:19:ILE:HG21	3:A:25:ARG:NH1	0.59	2.13	9	7
3:A:111:CYS:O	3:A:115:ASN:N	0.59	2.36	10	16
2:C:421:DT:P	3:A:130:ARG:HH22	0.59	2.20	6	2
3:A:61:ASN:H	3:A:61:ASN:ND2	0.58	1.95	19	1
3:A:39:ARG:CG	3:A:39:ARG:HH11	0.58	2.12	19	2
2:C:420:DA:OP1	3:A:129:ASN:ND2	0.58	2.36	8	15
3:A:57:TYR:O	3:A:61:ASN:ND2	0.58	2.35	19	1
3:A:26:LYS:NZ	3:A:30:ASP:OD2	0.58	2.35	5	1
3:A:39:ARG:CG	3:A:39:ARG:NH1	0.57	2.67	19	2
3:A:20:ASN:ND2	3:A:22:ASP:OD1	0.57	2.37	4	1
3:A:14:ARG:NH1	3:A:18:GLU:OE2	0.57	2.37	1	1
3:A:66:ARG:HH21	3:A:80:GLU:CB	0.57	2.13	14	13
3:A:25:ARG:CG	3:A:25:ARG:NH1	0.57	2.67	4	4
3:A:22:ASP:OD1	3:A:25:ARG:N	0.57	2.36	1	1
3:A:66:ARG:NH2	3:A:80:GLU:OE1	0.57	2.36	6	1
3:A:129:ASN:HD22	3:A:130:ARG:N	0.57	1.96	1	6
3:A:82:ILE:HD11	3:A:95:ALA:HB2	0.57	1.76	7	13
3:A:39:ARG:NH1	3:A:39:ARG:CG	0.57	2.68	11	1
3:A:61:ASN:HD22	3:A:61:ASN:N	0.57	1.98	18	2
3:A:9:GLN:NE2	3:A:44:ASN:C	0.56	2.59	10	6
3:A:66:ARG:NE	3:A:80:GLU:OE1	0.56	2.36	6	1
3:A:20:ASN:ND2	3:A:25:ARG:NH1	0.56	2.52	15	1
3:A:130:ARG:CG	3:A:130:ARG:HH11	0.56	2.14	8	4
3:A:54:LEU:CD2	3:A:101:GLN:OE1	0.56	2.54	1	1
1:B:407:DT:OP2	3:A:45:ARG:NH2	0.55	2.40	10	1
2:C:419:DC:OP1	3:A:79:GLN:NE2	0.55	2.40	1	2
3:A:69:LEU:HD11	3:A:78:TRP:CH2	0.55	2.37	2	10
3:A:106:LEU:N	3:A:106:LEU:CD1	0.55	2.69	14	13
3:A:99:ARG:HH12	3:A:129:ASN:HD21	0.55	1.41	3	2
3:A:25:ARG:HH11	3:A:25:ARG:HG2	0.55	1.61	4	8
3:A:57:TYR:CE2	3:A:61:ASN:ND2	0.55	2.75	11	2
3:A:25:ARG:NH1	3:A:25:ARG:CG	0.54	2.69	8	4
3:A:126:ILE:O	3:A:129:ASN:OD1	0.54	2.24	4	9
3:A:25:ARG:CG	3:A:25:ARG:HH11	0.54	2.16	8	4
3:A:44:ASN:O	3:A:45:ARG:CZ	0.54	2.56	1	1
3:A:63:VAL:HG21	3:A:102:TYR:CD2	0.54	2.37	13	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:420:DA:OP1	3:A:99:ARG:NH1	0.53	2.41	19	2
3:A:108:PRO:O	3:A:112:GLU:N	0.53	2.39	6	11
1:B:409:DG:C2	2:C:423:DA:C2	0.53	2.95	3	4
3:A:45:ARG:HH11	3:A:45:ARG:CG	0.53	2.16	5	3
3:A:20:ASN:C	3:A:20:ASN:HD22	0.53	2.06	12	2
2:C:421:DT:C7	3:A:96:LEU:HD22	0.53	2.34	7	3
3:A:103:MET:HG2	3:A:122:LEU:HD21	0.53	1.80	13	7
3:A:10:PHE:O	3:A:14:ARG:CG	0.53	2.57	15	1
3:A:78:TRP:HE1	3:A:99:ARG:HH12	0.53	1.45	10	1
3:A:20:ASN:C	3:A:20:ASN:ND2	0.53	2.62	12	2
3:A:78:TRP:O	3:A:82:ILE:N	0.53	2.37	13	17
3:A:107:TYR:CE2	3:A:111:CYS:SG	0.53	2.96	7	1
3:A:97:THR:HG22	3:A:101:GLN:NE2	0.52	2.18	8	1
1:B:402:DC:H6	1:B:402:DC:O5'	0.52	1.88	19	6
3:A:29:LEU:O	3:A:33:PHE:CD2	0.52	2.62	11	9
3:A:20:ASN:ND2	3:A:22:ASP:CG	0.52	2.62	4	1
3:A:9:GLN:N	3:A:9:GLN:CD	0.52	2.63	6	3
3:A:66:ARG:HG3	3:A:77:LEU:HD13	0.52	1.82	19	2
3:A:54:LEU:HD21	3:A:59:LEU:HD22	0.52	1.81	7	7
3:A:103:MET:HE2	3:A:126:ILE:HD11	0.52	1.82	9	1
3:A:19:ILE:HG21	3:A:25:ARG:HH12	0.52	1.64	2	5
3:A:14:ARG:CG	3:A:14:ARG:HH11	0.52	2.16	14	1
3:A:36:MET:CE	3:A:41:THR:O	0.52	2.57	14	4
3:A:45:ARG:CG	3:A:45:ARG:NH1	0.52	2.71	10	3
3:A:20:ASN:N	3:A:20:ASN:ND2	0.52	2.57	13	1
3:A:99:ARG:HH12	3:A:129:ASN:ND2	0.51	2.00	8	4
3:A:27:GLU:O	3:A:30:ASP:OD1	0.51	2.27	11	2
3:A:14:ARG:CG	3:A:14:ARG:NH1	0.51	2.70	14	1
3:A:17:TYR:OH	3:A:30:ASP:OD1	0.51	2.27	8	8
2:C:418:DA:C5	2:C:419:DC:C4	0.51	2.98	11	7
3:A:21:ASP:O	3:A:21:ASP:OD1	0.51	2.29	7	6
3:A:45:ARG:NH1	3:A:45:ARG:CG	0.51	2.72	14	2
3:A:103:MET:CE	3:A:122:LEU:HD11	0.51	2.36	6	1
3:A:110:GLU:CG	3:A:116:LEU:HD12	0.51	2.36	7	1
3:A:117:SER:OG	3:A:121:GLU:OE1	0.51	2.29	10	8
3:A:60:TYR:CZ	3:A:64:ILE:HD11	0.51	2.41	7	3
3:A:18:GLU:O	3:A:19:ILE:C	0.50	2.49	13	18
3:A:20:ASN:HD21	3:A:25:ARG:CD	0.50	2.19	15	1
3:A:23:PRO:O	3:A:27:GLU:OE1	0.50	2.29	19	1
3:A:79:GLN:H	3:A:79:GLN:CD	0.50	2.09	11	2
3:A:130:ARG:CG	3:A:130:ARG:NH1	0.50	2.71	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:412:DG:C6	2:C:418:DA:N6	0.50	2.80	13	2
3:A:33:PHE:CE1	3:A:43:ILE:HD12	0.50	2.42	17	2
1:B:409:DG:C5	1:B:410:DA:N6	0.50	2.79	8	1
3:A:126:ILE:CG2	3:A:130:ARG:HH22	0.50	2.20	8	1
3:A:124:ALA:O	3:A:127:ASP:OD1	0.50	2.29	18	1
3:A:25:ARG:HH22	3:A:55:ASP:CG	0.50	2.09	1	5
3:A:88:PRO:C	3:A:90:SER:H	0.50	2.10	2	14
1:B:408:DT:OP1	3:A:48:ILE:HG22	0.50	2.07	10	11
3:A:103:MET:CE	3:A:126:ILE:CD1	0.50	2.90	18	5
3:A:15:GLN:NE2	3:A:18:GLU:OE1	0.49	2.45	20	1
3:A:14:ARG:O	3:A:18:GLU:OE1	0.49	2.29	13	1
3:A:72:VAL:O	3:A:76:LYS:CA	0.49	2.60	2	20
3:A:19:ILE:O	3:A:20:ASN:OD1	0.49	2.31	11	6
3:A:110:GLU:O	3:A:110:GLU:OE1	0.49	2.30	18	1
1:B:408:DT:OP2	3:A:48:ILE:O	0.49	2.30	5	20
3:A:108:PRO:O	3:A:112:GLU:CB	0.49	2.60	15	9
3:A:96:LEU:O	3:A:100:THR:OG1	0.49	2.29	6	6
1:B:401:DC:O5'	1:B:401:DC:C6	0.49	2.51	11	2
3:A:45:ARG:CG	3:A:45:ARG:HH11	0.49	2.18	14	2
3:A:20:ASN:ND2	3:A:25:ARG:HH11	0.49	2.02	15	1
3:A:9:GLN:OE1	3:A:43:ILE:O	0.49	2.31	13	2
3:A:35:PHE:CD1	3:A:35:PHE:O	0.49	2.65	13	1
3:A:97:THR:HG22	3:A:101:GLN:HE22	0.49	1.67	8	1
3:A:14:ARG:NH2	3:A:18:GLU:OE2	0.49	2.46	16	1
3:A:73:ILE:CD1	3:A:122:LEU:CD1	0.48	2.91	16	7
2:C:419:DC:P	3:A:79:GLN:NE2	0.48	2.87	1	2
2:C:421:DT:C4	2:C:422:DC:C4	0.48	3.02	14	7
3:A:88:PRO:C	3:A:90:SER:N	0.48	2.67	4	11
3:A:27:GLU:C	3:A:30:ASP:OD1	0.48	2.52	11	1
3:A:19:ILE:HG21	3:A:25:ARG:NH2	0.48	2.23	11	1
3:A:57:TYR:CZ	3:A:61:ASN:ND2	0.48	2.80	20	2
3:A:49:MET:O	3:A:50:ALA:CB	0.48	2.62	17	6
3:A:60:TYR:CE2	3:A:64:ILE:HD11	0.48	2.44	18	1
3:A:88:PRO:O	3:A:90:SER:N	0.48	2.46	13	11
3:A:25:ARG:NH1	3:A:29:LEU:HD11	0.47	2.24	18	4
2:C:421:DT:O4	3:A:93:SER:OG	0.47	2.32	9	2
2:C:421:DT:C7	3:A:96:LEU:CD2	0.47	2.92	16	8
3:A:32:LEU:HD23	3:A:56:LEU:HD13	0.47	1.85	14	1
3:A:69:LEU:N	3:A:110:GLU:OE2	0.47	2.43	6	2
3:A:102:TYR:CE1	3:A:110:GLU:OE1	0.47	2.68	1	2
1:B:409:DG:C6	1:B:410:DA:N6	0.47	2.82	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:45:ARG:O	3:A:45:ARG:CD	0.47	2.62	18	2
3:A:80:GLU:O	3:A:84:GLY:N	0.47	2.44	10	5
3:A:45:ARG:CG	3:A:45:ARG:O	0.47	2.63	13	1
2:C:418:DA:C2	2:C:419:DC:C2	0.47	3.02	8	5
3:A:64:ILE:HD12	3:A:110:GLU:OE1	0.47	2.10	19	1
3:A:99:ARG:CZ	3:A:99:ARG:CB	0.46	2.93	10	3
3:A:105:TYR:C	3:A:106:LEU:HD12	0.46	2.31	17	4
3:A:16:LEU:HA	3:A:19:ILE:HD12	0.46	1.86	10	2
3:A:55:ASP:N	3:A:55:ASP:OD1	0.46	2.48	1	3
3:A:78:TRP:O	3:A:81:ILE:N	0.46	2.49	3	6
3:A:129:ASN:OD1	3:A:129:ASN:C	0.46	2.53	11	4
3:A:62:LEU:CA	3:A:66:ARG:NH1	0.46	2.78	4	3
3:A:45:ARG:NH2	3:A:105:TYR:CZ	0.46	2.83	18	1
3:A:19:ILE:CG2	3:A:25:ARG:NH1	0.46	2.79	1	3
3:A:14:ARG:NH1	3:A:14:ARG:CG	0.46	2.78	1	1
3:A:18:GLU:N	3:A:18:GLU:CD	0.46	2.68	13	1
3:A:103:MET:HE1	3:A:126:ILE:HD11	0.46	1.86	6	1
3:A:96:LEU:HD12	3:A:99:ARG:NH2	0.46	2.25	20	1
3:A:85:LEU:CD2	3:A:85:LEU:N	0.46	2.78	4	1
3:A:48:ILE:HG23	3:A:52:SER:N	0.46	2.26	7	6
3:A:66:ARG:CG	3:A:77:LEU:HD13	0.46	2.41	9	7
3:A:61:ASN:N	3:A:61:ASN:ND2	0.46	2.63	18	2
3:A:107:TYR:OH	3:A:118:THR:C	0.46	2.54	10	4
3:A:32:LEU:O	3:A:36:MET:CG	0.46	2.64	15	1
2:C:421:DT:OP2	3:A:130:ARG:NH2	0.46	2.49	6	2
3:A:19:ILE:O	3:A:20:ASN:CG	0.46	2.54	11	1
3:A:111:CYS:O	3:A:115:ASN:CA	0.45	2.65	12	10
3:A:60:TYR:O	3:A:61:ASN:C	0.45	2.54	17	8
1:B:409:DG:N2	2:C:423:DA:C2	0.45	2.84	3	2
3:A:20:ASN:N	3:A:20:ASN:HD22	0.45	2.10	13	2
1:B:408:DT:OP1	3:A:48:ILE:C	0.45	2.55	13	6
3:A:19:ILE:HD13	3:A:55:ASP:OD1	0.45	2.11	11	1
3:A:130:ARG:HB3	3:A:130:ARG:HH11	0.45	1.72	11	1
3:A:60:TYR:O	3:A:63:VAL:N	0.45	2.50	18	2
1:B:408:DT:OP1	3:A:48:ILE:O	0.45	2.35	14	11
3:A:107:TYR:N	3:A:108:PRO:HD2	0.45	2.27	17	8
3:A:78:TRP:HE1	3:A:99:ARG:NH1	0.45	2.09	10	1
2:C:419:DC:OP2	3:A:79:GLN:NE2	0.45	2.49	8	2
3:A:60:TYR:CE1	3:A:64:ILE:CD1	0.45	2.91	5	1
3:A:64:ILE:HG23	3:A:116:LEU:HD11	0.45	1.88	5	1
3:A:69:LEU:HD13	3:A:102:TYR:CG	0.45	2.47	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:85:LEU:C	3:A:86:HIS:CD2	0.45	2.90	10	1
3:A:62:LEU:HD13	3:A:81:ILE:HA	0.45	1.89	13	1
3:A:50:ALA:H	3:A:91:ILE:HD11	0.45	1.71	17	1
3:A:70:VAL:HG22	3:A:122:LEU:HA	0.45	1.88	1	1
3:A:78:TRP:O	3:A:79:GLN:C	0.45	2.55	8	19
3:A:72:VAL:HG12	3:A:78:TRP:CE2	0.45	2.46	8	7
3:A:111:CYS:SG	3:A:117:SER:O	0.45	2.75	10	3
3:A:62:LEU:O	3:A:65:ALA:HB3	0.45	2.11	17	1
3:A:103:MET:SD	3:A:126:ILE:CD1	0.45	3.05	8	4
3:A:59:LEU:HD13	3:A:98:LEU:HD22	0.45	1.88	5	1
3:A:127:ASP:OD1	3:A:130:ARG:NH2	0.45	2.50	10	1
3:A:20:ASN:ND2	3:A:20:ASN:N	0.45	2.63	15	1
3:A:83:LYS:O	3:A:86:HIS:N	0.45	2.48	1	3
3:A:45:ARG:HH11	3:A:45:ARG:HB3	0.45	1.72	19	1
3:A:123:GLN:NE2	3:A:126:ILE:HD12	0.44	2.27	6	1
3:A:20:ASN:OD1	3:A:20:ASN:C	0.44	2.55	8	1
3:A:79:GLN:H	3:A:79:GLN:NE2	0.44	2.10	11	1
1:B:407:DT:P	3:A:45:ARG:HH11	0.44	2.35	18	1
2:C:421:DT:H73	3:A:96:LEU:CD2	0.44	2.43	17	1
3:A:64:ILE:CD1	3:A:110:GLU:OE1	0.44	2.65	19	1
3:A:130:ARG:NH1	3:A:130:ARG:CG	0.44	2.80	11	1
3:A:107:TYR:O	3:A:111:CYS:SG	0.44	2.76	7	1
3:A:45:ARG:HH11	3:A:45:ARG:CB	0.44	2.25	19	1
3:A:44:ASN:O	3:A:45:ARG:CD	0.43	2.66	1	1
3:A:103:MET:HG3	3:A:122:LEU:HD21	0.43	1.90	4	4
3:A:19:ILE:CG2	3:A:25:ARG:HH12	0.43	2.25	16	2
3:A:13:VAL:HG23	3:A:33:PHE:CE2	0.43	2.47	9	1
3:A:49:MET:SD	3:A:91:ILE:HD13	0.43	2.54	16	1
3:A:60:TYR:CE2	3:A:64:ILE:CD1	0.43	3.01	18	1
3:A:22:ASP:C	3:A:22:ASP:OD1	0.43	2.57	9	1
3:A:79:GLN:NE2	3:A:79:GLN:H	0.43	2.12	10	1
3:A:114:LYS:HG2	3:A:116:LEU:HD21	0.43	1.91	16	2
3:A:17:TYR:OH	3:A:30:ASP:CG	0.43	2.57	19	1
3:A:110:GLU:CD	3:A:110:GLU:C	0.43	2.76	19	1
1:B:412:DG:N2	2:C:420:DA:C2	0.43	2.87	3	1
2:C:421:DT:P	3:A:130:ARG:HH12	0.43	2.37	12	1
3:A:48:ILE:HG23	3:A:52:SER:O	0.43	2.12	17	2
3:A:34:SER:OG	3:A:35:PHE:N	0.43	2.52	1	1
3:A:101:GLN:CG	3:A:102:TYR:N	0.43	2.81	1	1
2:C:421:DT:H72	3:A:96:LEU:HD22	0.43	1.90	11	1
3:A:14:ARG:HH11	3:A:14:ARG:HG2	0.43	1.74	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:105:TYR:CD1	3:A:105:TYR:N	0.43	2.87	8	3
3:A:25:ARG:NH2	3:A:55:ASP:CG	0.42	2.73	19	2
3:A:19:ILE:HD13	3:A:25:ARG:HH22	0.42	1.70	1	1
3:A:37:GLN:OE1	3:A:37:GLN:C	0.42	2.57	1	1
3:A:103:MET:HE1	3:A:126:ILE:CD1	0.42	2.45	12	1
3:A:63:VAL:CG2	3:A:102:TYR:CE2	0.42	2.97	13	1
3:A:39:ARG:NE	3:A:39:ARG:HA	0.42	2.30	14	1
3:A:127:ASP:OD1	3:A:127:ASP:C	0.42	2.58	18	1
3:A:74:ASN:OD1	3:A:125:ALA:CB	0.42	2.66	3	1
3:A:30:ASP:CG	3:A:31:ASP:N	0.42	2.73	17	1
3:A:13:VAL:O	3:A:16:LEU:N	0.42	2.51	2	2
3:A:19:ILE:CD1	3:A:25:ARG:NH2	0.42	2.83	2	1
3:A:130:ARG:HH11	3:A:130:ARG:HB3	0.42	1.75	13	2
3:A:107:TYR:N	3:A:108:PRO:HD3	0.42	2.29	11	2
3:A:69:LEU:HD11	3:A:78:TRP:HH2	0.42	1.73	2	3
3:A:21:ASP:OD1	3:A:21:ASP:C	0.41	2.57	7	3
3:A:72:VAL:HG12	3:A:78:TRP:NE1	0.41	2.30	16	2
3:A:123:GLN:HA	3:A:126:ILE:HD12	0.41	1.93	9	1
3:A:39:ARG:NH1	3:A:108:PRO:CB	0.41	2.84	14	2
3:A:107:TYR:OH	3:A:119:PRO:CD	0.41	2.69	14	1
3:A:103:MET:O	3:A:107:TYR:CB	0.41	2.69	12	1
3:A:49:MET:SD	3:A:87:LEU:CD2	0.41	3.09	1	1
3:A:64:ILE:CD1	3:A:110:GLU:OE2	0.41	2.68	18	1
3:A:79:GLN:OE1	3:A:83:LYS:NZ	0.41	2.53	8	1
3:A:72:VAL:HG12	3:A:78:TRP:CD1	0.41	2.50	12	1
3:A:61:ASN:ND2	3:A:61:ASN:N	0.41	2.66	19	1
3:A:31:ASP:OD2	3:A:109:TYR:OH	0.41	2.35	1	1
3:A:16:LEU:HB3	3:A:29:LEU:HD13	0.41	1.92	10	1
3:A:130:ARG:HH11	3:A:130:ARG:CB	0.41	2.29	13	1
3:A:20:ASN:ND2	3:A:25:ARG:HD3	0.41	2.29	15	1
3:A:22:ASP:OD1	3:A:22:ASP:C	0.41	2.58	16	1
3:A:16:LEU:HD13	3:A:29:LEU:HD22	0.41	1.92	10	1
3:A:62:LEU:O	3:A:66:ARG:CD	0.41	2.69	15	1
1:B:406:DA:C5	1:B:407:DT:C4	0.41	3.08	17	1
3:A:70:VAL:HG12	3:A:74:ASN:OD1	0.40	2.16	1	1
3:A:79:GLN:CD	3:A:79:GLN:N	0.40	2.75	11	1
3:A:9:GLN:NE2	3:A:45:ARG:N	0.40	2.69	7	1
3:A:79:GLN:NE2	3:A:79:GLN:N	0.40	2.68	11	1
3:A:18:GLU:O	3:A:20:ASN:N	0.40	2.54	13	1
3:A:16:LEU:CD1	3:A:46:LEU:HD13	0.40	2.46	15	1
3:A:35:PHE:CD1	3:A:38:LYS:NZ	0.40	2.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:99:ARG:CZ	3:A:129:ASN:ND2	0.40	2.85	2	1
3:A:130:ARG:HH11	3:A:130:ARG:CG	0.40	2.28	11	1
3:A:130:ARG:NH1	3:A:130:ARG:HG2	0.40	2.31	12	1
3:A:110:GLU:OE1	3:A:111:CYS:N	0.40	2.55	2	1
3:A:66:ARG:HH21	3:A:80:GLU:HB3	0.40	1.76	5	1
3:A:94:ALA:O	3:A:95:ALA:C	0.40	2.60	14	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	
3	A	122/139 (88%)	112±1 (92±1%)	9±1 (7±1%)	1±1 (1±1%)	21	69
All	All	2440/2780 (88%)	2241 (92%)	177 (7%)	22 (1%)	21	69

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	89	SER	9
3	A	23	PRO	7
3	A	55	ASP	5
3	A	19	ILE	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	
3	A	110/123 (89%)	105±2 (96±1%)	5±2 (4±1%)	31	80
All	All	2200/2460 (89%)	2101 (96%)	99 (4%)	31	80

All 28 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)
3	A	129	ASN	11
3	A	45	ARG	9
3	A	20	ASN	9
3	A	22	ASP	7
3	A	25	ARG	6
3	A	39	ARG	6
3	A	15	GLN	6
3	A	100	THR	5
3	A	13	VAL	4
3	A	130	ARG	4
3	A	14	ARG	3
3	A	115	ASN	3
3	A	38	LYS	3
3	A	24	LYS	3
3	A	75	LYS	2
3	A	11	LYS	2
3	A	46	LEU	2
3	A	114	LYS	2
3	A	35	PHE	2
3	A	111	CYS	2
3	A	101	GLN	1
3	A	109	TYR	1
3	A	110	GLU	1
3	A	66	ARG	1
3	A	18	GLU	1
3	A	30	ASP	1
3	A	104	LYS	1
3	A	103	MET	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

No chemical shift data were provided