Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 07:46 PM EST

PDB ID	:	2O8K
Title	:	NMR Structure of the Sigma-54 RpoN Domain Bound to the-24 Promoter Element
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Deposited on	:	2006-12-12

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:

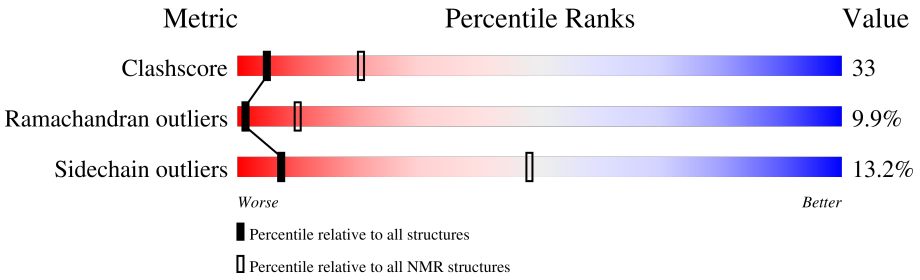
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	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	14	21% 50% 29%
2	C	14	21% 79%
3	A	63	29% 57% 6% • 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:16-A:74 (59)	0.19	6

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 4 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1969 atoms, of which 878 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	14	444	137	163	43	88	13	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	C	14	444	137	157	61	76	13	0

- Molecule 3 is a protein called RNA polymerase sigma factor RpoN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	A	63	1081	327	558	98	95	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	HIS	-	cloning artifact	UNP O66858
A	15	MET	-	cloning artifact	UNP O66858

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

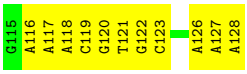
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'

Chain B:

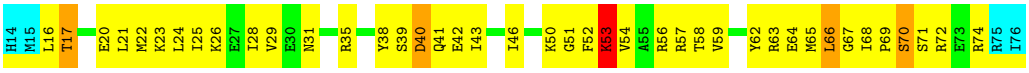
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

Chain A:



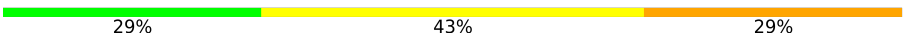
4.2 Scores per residue for each member of the ensemble

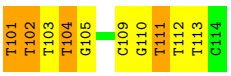
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

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

Chain B:



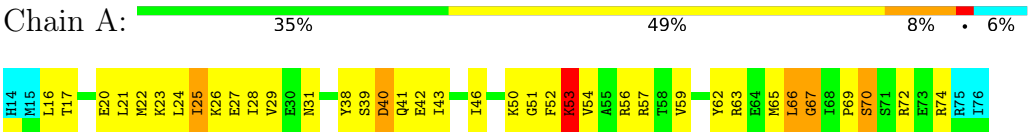


• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:

• Molecule 3: RNA polymerase sigma factor RpoN

Chain A:



4.2.2 Score per residue for model 2

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

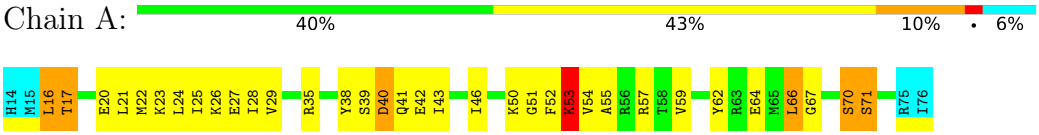
Chain B:

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

Chain C:

• Molecule 3: RNA polymerase sigma factor RpoN

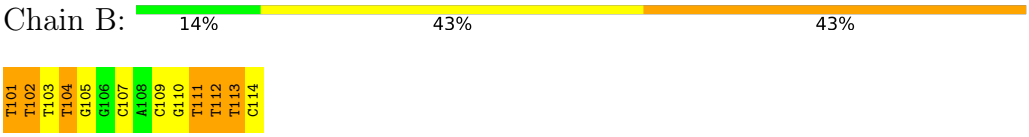
Chain A:



4.2.3 Score per residue for model 3

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

Chain B:

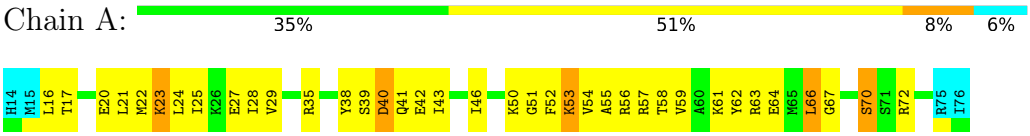


• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:

• Molecule 3: RNA polymerase sigma factor RpoN

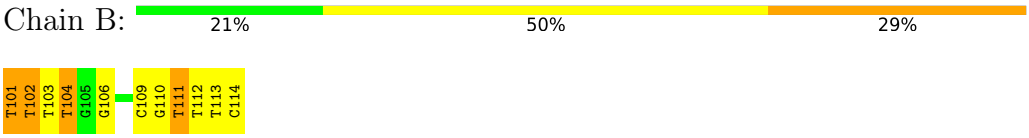
Chain A:



4.2.4 Score per residue for model 4

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

Chain B:

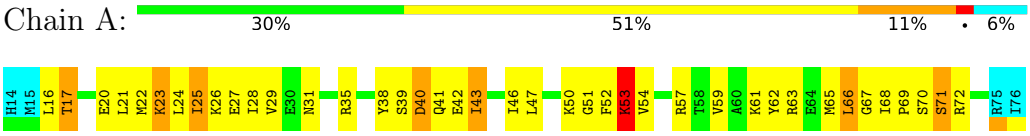


• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:

• Molecule 3: RNA polymerase sigma factor RpoN

Chain A:



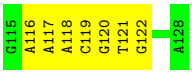
4.2.5 Score per residue for model 5

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

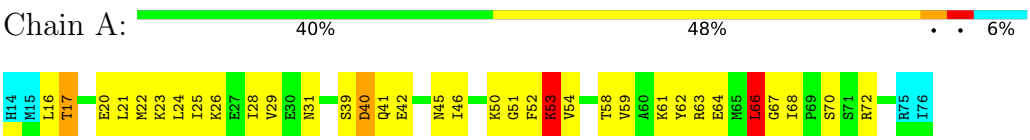
Chain B:

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

Chain C:

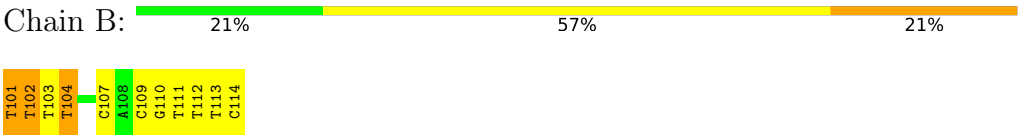


• Molecule 3: RNA polymerase sigma factor RpoN



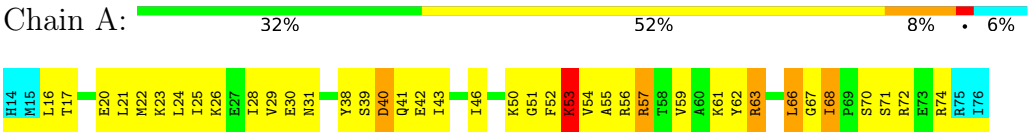
4.2.6 Score per residue for model 6 (medoid)

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



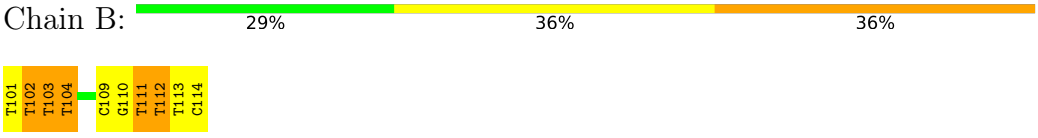
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

• Molecule 3: RNA polymerase sigma factor RpoN



4.2.7 Score per residue for model 7

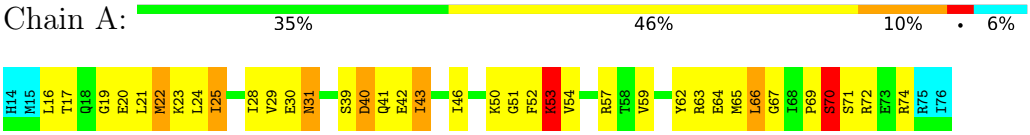
• Molecule 1: 5'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'



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

• Molecule 3: RNA polymerase sigma factor RpoN

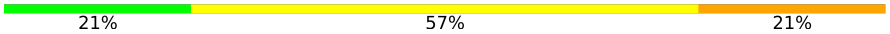
Chain A:

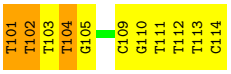


4.2.8 Score per residue for model 8

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

Chain B:





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

Chain C:

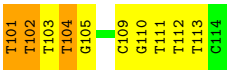
• Molecule 3: RNA polymerase sigma factor RpoN

Chain A:

4.2.9 Score per residue for model 9

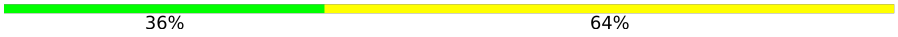
• Molecule 1: 5'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'

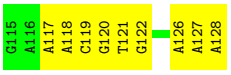
Chain B:



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

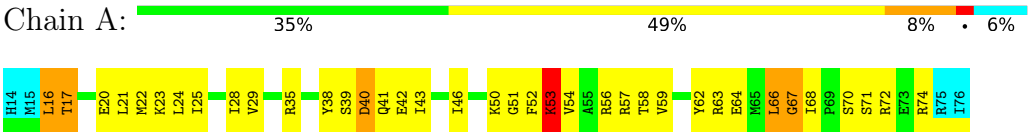
Chain C:





• Molecule 3: RNA polymerase sigma factor RpoN

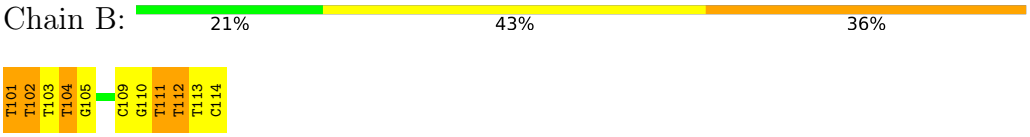
Chain A:



4.2.10 Score per residue for model 10

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

Chain B:

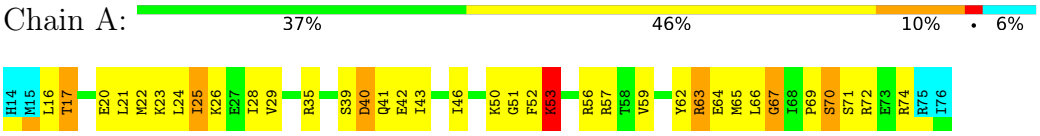


• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:

• Molecule 3: RNA polymerase sigma factor RpoN

Chain A:



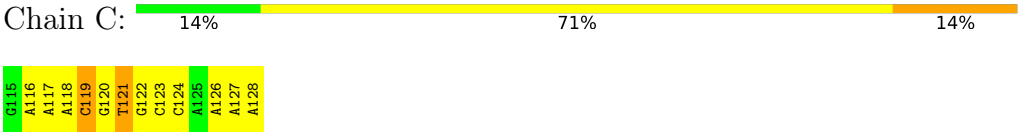
4.2.11 Score per residue for model 11

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

Chain B:

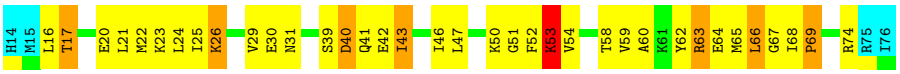
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

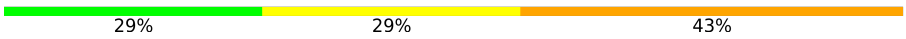
Chain A:

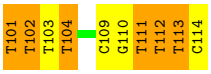


4.2.12 Score per residue for model 12

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

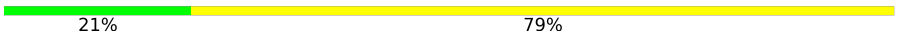
Chain B:





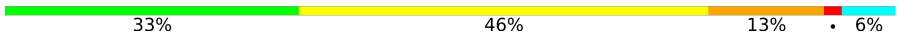
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

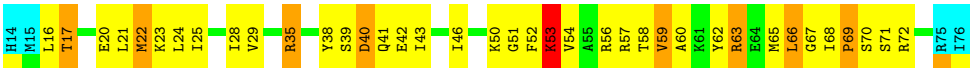
Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

Chain A:

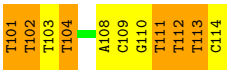




4.2.13 Score per residue for model 13

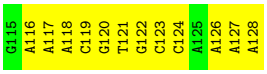
• Molecule 1: 5'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'

Chain B:



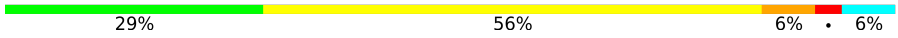
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

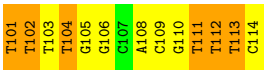
Chain A:



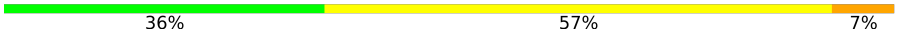
4.2.14 Score per residue for model 14

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

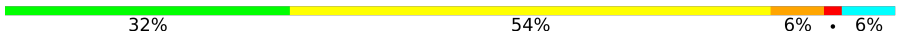
Chain B: 



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

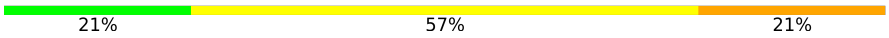
Chain C: 

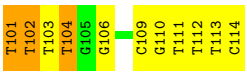
• Molecule 3: RNA polymerase sigma factor RpoN

Chain A: 

4.2.15 Score per residue for model 15

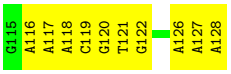
• Molecule 1: 5'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'

Chain B: 



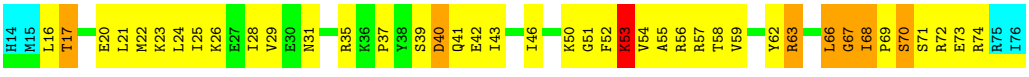
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C: 



• Molecule 3: RNA polymerase sigma factor RpoN

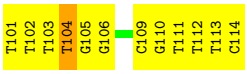
Chain A: 



4.2.16 Score per residue for model 16

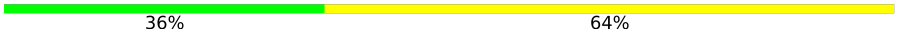
• Molecule 1: 5'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'

Chain B:



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

Chain C:



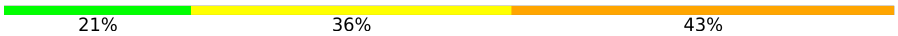
• Molecule 3: RNA polymerase sigma factor RpoN

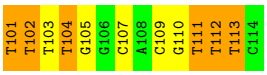
Chain A:

4.2.17 Score per residue for model 17

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

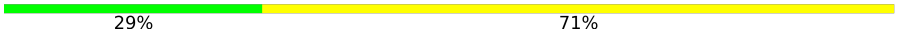
Chain B:





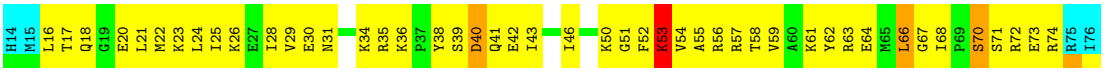
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

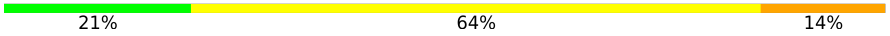
Chain A:

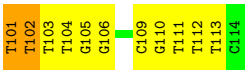


4.2.18 Score per residue for model 18

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

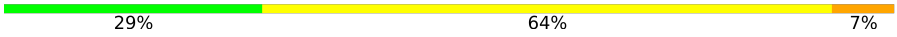
Chain B:





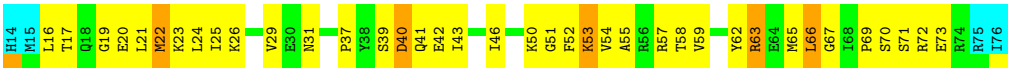
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

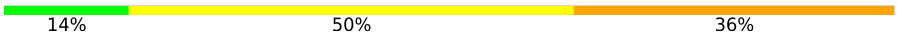
Chain A:



4.2.19 Score per residue for model 19

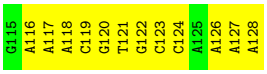
• Molecule 1: 5'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'

Chain B:



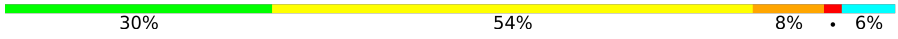
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

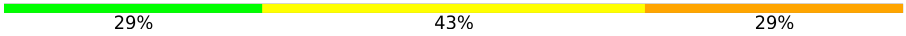
Chain A:



4.2.20 Score per residue for model 20

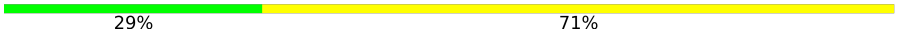
• Molecule 1: 5'-D(*TP*TP*TP*TP*GP*GP*CP*AP*CP*GP*TP*TP*TP*C)-3'

Chain B:



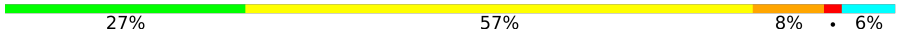
• Molecule 2: 5'-D(*GP*AP*AP*AP*CP*GP*TP*GP*CP*CP*AP*AP*AP*A)-3'

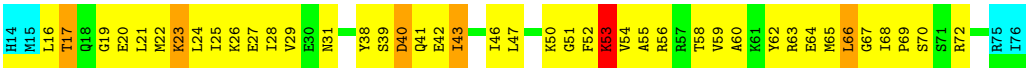
Chain C:



• Molecule 3: RNA polymerase sigma factor RpoN

Chain A:





5 Refinement protocol and experimental data overview

The models were refined using the following method: *docking, rigid-body minimization, simulated annealing.*

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *20 structures with lowest energy and no restraint violations greater than 0.5 A and 5 degrees for distance and dihedral restraints, respectively.*

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

Software name	Classification	Version
CYANA	structure solution	2.1
X-PLOR	refinement	2.14

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	1.37±0.02	1±2/312 (0.5± 0.5%)	1.64±0.01	10±1/480 (2.0± 0.2%)
2	C	1.20±0.02	0±0/324 (0.1± 0.1%)	1.51±0.02	2±0/498 (0.4± 0.1%)
3	A	0.74±0.00	0±0/490 (0.0± 0.0%)	0.75±0.01	0±0/652 (0.0± 0.0%)
All	All	1.08	34/22520 (0.2%)	1.31	240/32600 (0.7%)

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	111	DT	C5-C7	5.63	1.53	1.50	20	7
2	C	121	DT	C5-C7	5.48	1.53	1.50	4	4
1	B	101	DT	C5-C7	5.45	1.53	1.50	9	5
1	B	112	DT	C5-C7	5.41	1.53	1.50	9	7
1	B	102	DT	C5-C7	5.29	1.53	1.50	20	2
1	B	103	DT	C5-C7	5.28	1.53	1.50	9	7
1	B	104	DT	C5-C7	5.15	1.53	1.50	20	1
2	C	119	DC	N1-C6	-5.06	1.34	1.37	11	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	C	121	DT	C6-C5-C7	-6.63	118.92	122.90	20	20
1	B	113	DT	C6-C5-C7	-6.19	119.18	122.90	16	20
1	B	103	DT	C6-C5-C7	-6.12	119.23	122.90	19	20
1	B	104	DT	C6-C5-C7	-5.94	119.33	122.90	9	20
2	C	121	DT	C4-C5-C6	5.91	121.55	118.00	12	20
1	B	102	DT	C6-C5-C7	-5.78	119.43	122.90	5	20
1	B	114	DC	C6-N1-C2	5.61	122.55	120.30	8	14
1	B	111	DT	C6-C5-C7	-5.59	119.55	122.90	16	15
1	B	101	DT	C6-C5-C7	-5.56	119.56	122.90	13	19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	112	DT	C6-C5-C7	-5.55	119.57	122.90	13	19
1	B	103	DT	C4-C5-C6	5.46	121.28	118.00	18	17
2	C	122	DG	N7-C8-N9	5.38	115.79	113.10	14	4
1	B	104	DT	C4-C5-C6	5.34	121.21	118.00	7	10
1	B	113	DT	C4-C5-C6	5.30	121.18	118.00	12	20
1	B	102	DT	C4-C5-C6	5.20	121.12	118.00	9	2

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	281	163	163	12±4
2	C	287	157	157	16±5
3	A	485	515	515	45±5
All	All	21060	16700	16700	1253

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:ILE:HD11	3:A:66:LEU:HD13	0.90	1.44	9	17
3:A:25:ILE:HD11	3:A:66:LEU:CD1	0.76	2.11	5	14
3:A:17:THR:HG23	3:A:20:GLU:OE2	0.76	1.81	14	8
3:A:25:ILE:O	3:A:29:VAL:HG22	0.74	1.82	4	1
3:A:23:LYS:C	3:A:24:LEU:HD22	0.72	2.05	20	20
3:A:20:GLU:O	3:A:24:LEU:HD23	0.71	1.86	8	10
1:B:105:DG:C6	3:A:57:ARG:NH2	0.69	2.60	19	1
3:A:17:THR:HG23	3:A:20:GLU:OE1	0.69	1.87	2	6
2:C:123:DC:N4	3:A:57:ARG:HE	0.67	1.87	19	4
1:B:104:DT:C6	3:A:56:ARG:NH2	0.65	2.63	3	3
2:C:123:DC:N4	3:A:57:ARG:NE	0.65	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:117:DA:C6	2:C:118:DA:C6	0.64	2.86	12	20
3:A:16:LEU:HD12	3:A:21:LEU:HD23	0.64	1.68	8	20
1:B:105:DG:C5	3:A:57:ARG:NH2	0.64	2.64	18	1
2:C:117:DA:N6	2:C:118:DA:N6	0.64	2.46	20	20
3:A:25:ILE:O	3:A:29:VAL:HG23	0.64	1.93	12	19
3:A:39:SER:O	3:A:42:GLU:N	0.64	2.31	1	20
2:C:116:DA:C6	2:C:117:DA:C6	0.64	2.86	12	13
3:A:57:ARG:N	3:A:57:ARG:HE	0.63	1.90	6	1
2:C:122:DG:C6	2:C:123:DC:N4	0.63	2.67	19	7
1:B:105:DG:P	3:A:63:ARG:HH12	0.62	2.16	11	3
3:A:41:GLN:NE2	3:A:41:GLN:O	0.62	2.33	6	13
3:A:31:ASN:ND2	3:A:31:ASN:O	0.62	2.32	19	3
3:A:60:ALA:O	3:A:63:ARG:NH1	0.62	2.31	14	5
3:A:52:PHE:O	3:A:54:VAL:N	0.61	2.33	17	19
2:C:123:DC:H41	3:A:57:ARG:NE	0.61	1.93	17	3
2:C:126:DA:N6	2:C:127:DA:N6	0.61	2.49	12	14
3:A:22:MET:HG3	3:A:66:LEU:HD21	0.61	1.71	18	16
3:A:68:ILE:CG2	3:A:71:SER:H	0.61	2.09	13	2
3:A:63:ARG:NH2	3:A:69:PRO:O	0.61	2.34	11	9
3:A:67:GLY:O	3:A:74:ARG:NH2	0.60	2.35	15	4
1:B:109:DC:C4	1:B:110:DG:C6	0.60	2.90	8	19
1:B:110:DG:C2	2:C:120:DG:C2	0.60	2.89	14	1
3:A:39:SER:O	3:A:41:GLN:N	0.60	2.35	8	18
3:A:63:ARG:NH1	3:A:69:PRO:O	0.60	2.35	1	3
3:A:30:GLU:OE2	3:A:74:ARG:NH1	0.59	2.35	11	2
1:B:104:DT:OP1	3:A:63:ARG:NH1	0.59	2.35	9	3
3:A:40:ASP:OD1	3:A:41:GLN:N	0.59	2.36	14	7
3:A:40:ASP:OD1	3:A:56:ARG:NH2	0.59	2.34	9	1
3:A:40:ASP:OD2	3:A:41:GLN:N	0.59	2.35	19	8
3:A:30:GLU:OE1	3:A:74:ARG:NH1	0.59	2.36	13	2
3:A:42:GLU:N	3:A:42:GLU:OE2	0.59	2.36	12	1
2:C:120:DG:OP2	3:A:62:TYR:CZ	0.58	2.56	15	9
3:A:62:TYR:O	3:A:65:MET:N	0.58	2.36	20	10
2:C:120:DG:P	3:A:62:TYR:OH	0.58	2.60	5	19
3:A:24:LEU:HD22	3:A:24:LEU:N	0.58	2.12	4	20
3:A:22:MET:O	3:A:66:LEU:HD21	0.58	1.97	7	4
1:B:108:DA:C2	1:B:109:DC:C2	0.58	2.92	14	1
3:A:57:ARG:N	3:A:57:ARG:NE	0.58	2.52	6	1
3:A:42:GLU:N	3:A:42:GLU:OE1	0.58	2.37	1	2
1:B:106:DG:C6	1:B:107:DC:C4	0.58	2.92	19	1
3:A:41:GLN:CD	3:A:42:GLU:N	0.58	2.58	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:ILE:O	3:A:29:VAL:CG2	0.58	2.52	12	19
3:A:41:GLN:OE1	3:A:56:ARG:NH2	0.58	2.33	20	4
3:A:70:SER:C	3:A:72:ARG:H	0.57	2.02	7	17
1:B:107:DC:H41	3:A:61:LYS:NZ	0.57	1.97	6	4
3:A:40:ASP:N	3:A:63:ARG:NH1	0.57	2.52	17	1
2:C:120:DG:P	3:A:58:THR:CG2	0.57	2.93	8	3
2:C:120:DG:P	3:A:62:TYR:HH	0.57	2.22	17	11
2:C:127:DA:N1	2:C:128:DA:C6	0.56	2.73	1	12
3:A:20:GLU:O	3:A:24:LEU:CD2	0.56	2.53	19	8
3:A:22:MET:HG3	3:A:66:LEU:HD11	0.56	1.76	14	11
3:A:26:LYS:H	3:A:26:LYS:CD	0.56	2.13	8	1
2:C:122:DG:OP2	3:A:57:ARG:NH1	0.56	2.39	10	3
1:B:106:DG:O6	3:A:57:ARG:NE	0.56	2.39	18	2
3:A:56:ARG:NH2	3:A:57:ARG:HH12	0.56	1.99	15	1
1:B:112:DT:C5	1:B:113:DT:H73	0.56	2.35	17	6
2:C:122:DG:C5	2:C:123:DC:C4	0.56	2.93	3	4
2:C:120:DG:OP2	3:A:62:TYR:CE1	0.56	2.58	9	10
3:A:21:LEU:HD11	3:A:62:TYR:CD2	0.56	2.36	19	13
2:C:120:DG:P	3:A:62:TYR:CZ	0.56	2.99	18	2
1:B:105:DG:OP2	3:A:63:ARG:NH1	0.56	2.39	11	3
3:A:20:GLU:O	3:A:52:PHE:CE1	0.56	2.59	4	6
3:A:39:SER:O	3:A:40:ASP:C	0.55	2.45	3	20
3:A:63:ARG:HH21	3:A:70:SER:CA	0.55	2.15	7	1
3:A:70:SER:O	3:A:72:ARG:N	0.55	2.40	7	4
2:C:120:DG:OP1	3:A:62:TYR:CZ	0.55	2.59	8	2
1:B:106:DG:C6	3:A:57:ARG:CZ	0.55	2.90	19	1
1:B:107:DC:H41	3:A:61:LYS:HZ3	0.55	1.45	5	2
3:A:40:ASP:OD2	3:A:56:ARG:NE	0.55	2.35	16	1
3:A:24:LEU:O	3:A:28:ILE:HG23	0.55	2.02	4	5
2:C:122:DG:OP2	3:A:57:ARG:NH2	0.55	2.40	2	3
3:A:40:ASP:OD1	3:A:56:ARG:NE	0.55	2.36	3	1
3:A:30:GLU:CD	3:A:74:ARG:NH1	0.55	2.60	11	1
3:A:40:ASP:OD2	3:A:63:ARG:NE	0.54	2.40	13	1
3:A:63:ARG:CZ	3:A:69:PRO:O	0.54	2.55	15	4
3:A:63:ARG:NH1	3:A:70:SER:C	0.54	2.60	13	1
1:B:105:DG:P	3:A:63:ARG:NH2	0.54	2.81	1	1
3:A:52:PHE:O	3:A:53:LYS:C	0.54	2.45	6	20
3:A:70:SER:O	3:A:71:SER:CB	0.54	2.55	8	2
3:A:63:ARG:NH2	3:A:70:SER:C	0.54	2.60	17	2
1:B:105:DG:O6	3:A:56:ARG:NH1	0.54	2.40	3	3
3:A:65:MET:HG2	3:A:66:LEU:HD12	0.54	1.80	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:108:DA:C2	1:B:109:DC:N3	0.54	2.76	14	3
1:B:103:DT:O4'	3:A:72:ARG:NH2	0.54	2.41	19	1
1:B:109:DC:N4	1:B:110:DG:O6	0.54	2.41	20	19
2:C:123:DC:N4	2:C:124:DC:N4	0.54	2.56	17	6
1:B:110:DG:N7	1:B:111:DT:H73	0.54	2.17	11	5
3:A:63:ARG:HH22	3:A:71:SER:CB	0.54	2.16	13	1
1:B:110:DG:N7	1:B:111:DT:C7	0.54	2.71	11	6
1:B:104:DT:O3'	3:A:63:ARG:NH2	0.53	2.41	1	1
1:B:104:DT:OP1	3:A:63:ARG:CZ	0.53	2.56	20	3
2:C:116:DA:C2	2:C:117:DA:C4	0.53	2.97	13	11
3:A:21:LEU:HD11	3:A:62:TYR:CD1	0.53	2.38	7	7
3:A:21:LEU:HD22	3:A:54:VAL:HG21	0.53	1.79	14	3
2:C:118:DA:C6	2:C:119:DC:N4	0.53	2.77	11	1
2:C:123:DC:H41	3:A:57:ARG:HE	0.53	1.47	1	3
1:B:112:DT:C4	1:B:113:DT:O4	0.53	2.62	17	4
3:A:43:ILE:CD1	3:A:63:ARG:NH1	0.53	2.72	7	1
3:A:24:LEU:N	3:A:24:LEU:CD2	0.53	2.71	4	17
3:A:20:GLU:O	3:A:52:PHE:CE2	0.53	2.62	2	7
3:A:26:LYS:O	3:A:30:GLU:CG	0.53	2.57	11	1
2:C:121:DT:OP2	3:A:54:VAL:HG23	0.53	2.04	14	1
2:C:121:DT:H71	3:A:58:THR:OG1	0.53	2.04	14	1
3:A:68:ILE:CG2	3:A:71:SER:N	0.52	2.72	13	1
3:A:54:VAL:CG2	3:A:55:ALA:N	0.52	2.72	18	8
1:B:104:DT:C5	3:A:56:ARG:NH2	0.52	2.78	16	3
1:B:104:DT:H71	3:A:56:ARG:NH1	0.52	2.20	10	2
2:C:119:DC:N4	2:C:120:DG:O6	0.52	2.43	9	16
3:A:46:ILE:HG22	3:A:50:LYS:CE	0.52	2.34	14	5
1:B:105:DG:OP1	3:A:64:GLU:CG	0.52	2.58	9	1
3:A:63:ARG:NH2	3:A:68:ILE:O	0.52	2.43	15	1
1:B:109:DC:N4	1:B:110:DG:C6	0.52	2.78	8	9
2:C:126:DA:C6	2:C:127:DA:N6	0.52	2.78	7	2
3:A:63:ARG:NE	3:A:69:PRO:O	0.52	2.43	11	1
1:B:104:DT:C3'	3:A:63:ARG:HH21	0.52	2.18	1	1
3:A:16:LEU:HD22	3:A:20:GLU:HB3	0.52	1.81	9	15
3:A:54:VAL:HG22	3:A:55:ALA:N	0.51	2.19	18	7
1:B:110:DG:C8	1:B:111:DT:C7	0.51	2.94	13	7
2:C:124:DC:H41	3:A:57:ARG:NH2	0.51	2.02	16	2
3:A:24:LEU:O	3:A:28:ILE:CG1	0.51	2.58	4	13
2:C:120:DG:OP2	3:A:58:THR:CG2	0.51	2.58	17	9
1:B:107:DC:N4	3:A:61:LYS:NZ	0.51	2.58	5	3
3:A:73:GLU:CD	3:A:74:ARG:N	0.51	2.63	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:117:DA:C6	2:C:118:DA:N6	0.51	2.79	12	13
2:C:127:DA:C6	2:C:128:DA:C6	0.51	2.99	20	15
1:B:104:DT:OP1	3:A:63:ARG:NE	0.51	2.44	19	2
3:A:63:ARG:HH12	3:A:71:SER:CB	0.51	2.19	13	1
3:A:40:ASP:H	3:A:63:ARG:NH1	0.51	2.03	17	1
1:B:106:DG:O6	3:A:57:ARG:CZ	0.51	2.59	19	2
3:A:40:ASP:CA	3:A:63:ARG:HH21	0.51	2.18	4	1
3:A:43:ILE:CD1	3:A:63:ARG:HH21	0.51	2.19	13	1
3:A:23:LYS:O	3:A:27:GLU:OE1	0.51	2.28	20	3
3:A:63:ARG:HE	3:A:63:ARG:C	0.51	2.10	15	2
1:B:101:DT:C5	1:B:102:DT:H73	0.50	2.41	11	17
2:C:121:DT:OP2	3:A:55:ALA:N	0.50	2.44	18	2
3:A:40:ASP:N	3:A:40:ASP:OD1	0.50	2.44	4	5
1:B:104:DT:H71	3:A:56:ARG:HH12	0.50	1.66	10	1
2:C:120:DG:OP2	3:A:62:TYR:CE2	0.50	2.64	4	4
3:A:63:ARG:O	3:A:68:ILE:O	0.50	2.30	15	10
3:A:57:ARG:NE	3:A:57:ARG:CA	0.50	2.75	6	1
3:A:30:GLU:OE1	3:A:74:ARG:CZ	0.50	2.59	11	2
2:C:123:DC:H42	3:A:57:ARG:HE	0.50	1.49	18	1
3:A:64:GLU:OE1	3:A:69:PRO:O	0.50	2.29	7	1
3:A:63:ARG:NH2	3:A:71:SER:OG	0.50	2.45	17	1
3:A:69:PRO:O	3:A:70:SER:CB	0.49	2.59	7	1
1:B:101:DT:C5	1:B:102:DT:C7	0.49	2.96	4	16
3:A:30:GLU:OE1	3:A:74:ARG:NE	0.49	2.44	7	1
3:A:70:SER:C	3:A:72:ARG:N	0.49	2.66	7	9
2:C:122:DG:OP2	3:A:57:ARG:CZ	0.49	2.60	2	1
1:B:105:DG:OP1	3:A:64:GLU:OE2	0.49	2.30	19	5
3:A:40:ASP:N	3:A:63:ARG:NH2	0.49	2.60	4	2
3:A:30:GLU:O	3:A:34:LYS:NZ	0.48	2.37	17	2
2:C:120:DG:OP2	3:A:62:TYR:OH	0.48	2.31	14	11
2:C:127:DA:C6	2:C:128:DA:N6	0.48	2.81	1	6
3:A:41:GLN:CD	3:A:41:GLN:C	0.48	2.72	11	6
3:A:63:ARG:HH12	3:A:71:SER:N	0.48	2.06	13	1
3:A:38:TYR:CD1	3:A:38:TYR:N	0.48	2.80	9	5
3:A:22:MET:CG	3:A:66:LEU:HD11	0.48	2.38	10	1
1:B:110:DG:C8	1:B:111:DT:H71	0.48	2.44	11	8
2:C:124:DC:H42	3:A:57:ARG:NH2	0.48	2.06	19	1
2:C:124:DC:H42	3:A:57:ARG:HH21	0.48	1.51	19	1
3:A:30:GLU:OE1	3:A:74:ARG:NH2	0.48	2.42	17	1
3:A:38:TYR:CD2	3:A:38:TYR:N	0.48	2.82	3	7
3:A:40:ASP:H	3:A:63:ARG:NH2	0.48	2.07	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:63:ARG:HH21	3:A:70:SER:C	0.48	2.11	17	2
3:A:16:LEU:HD22	3:A:20:GLU:CB	0.48	2.39	20	10
1:B:105:DG:P	3:A:63:ARG:HH22	0.48	2.31	18	1
2:C:123:DC:C4	2:C:124:DC:N4	0.47	2.82	18	5
3:A:46:ILE:HG22	3:A:50:LYS:HE2	0.47	1.85	14	5
2:C:122:DG:N7	3:A:57:ARG:NE	0.47	2.60	9	2
1:B:104:DT:OP1	3:A:70:SER:O	0.47	2.32	8	2
2:C:116:DA:N1	2:C:117:DA:C6	0.47	2.82	13	6
3:A:63:ARG:NH2	3:A:70:SER:O	0.47	2.47	7	1
3:A:60:ALA:O	3:A:63:ARG:CG	0.47	2.62	16	2
1:B:106:DG:C5	1:B:107:DC:C4	0.47	3.01	19	1
3:A:52:PHE:C	3:A:54:VAL:N	0.47	2.68	12	7
1:B:111:DT:C4	1:B:112:DT:C4	0.47	3.02	14	4
3:A:63:ARG:HH12	3:A:70:SER:C	0.47	2.12	13	1
3:A:39:SER:OG	3:A:42:GLU:OE1	0.47	2.33	17	2
1:B:105:DG:P	3:A:63:ARG:NH1	0.47	2.88	10	2
3:A:23:LYS:O	3:A:27:GLU:OE2	0.47	2.33	2	3
3:A:46:ILE:HG22	3:A:50:LYS:HE3	0.46	1.87	2	15
1:B:111:DT:C5	1:B:112:DT:H73	0.46	2.45	10	2
2:C:122:DG:C6	2:C:123:DC:C4	0.46	3.04	3	1
3:A:37:PRO:CB	3:A:71:SER:O	0.46	2.64	18	3
1:B:101:DT:C4	1:B:102:DT:C4	0.46	3.04	3	3
1:B:104:DT:OP2	3:A:40:ASP:N	0.46	2.48	11	3
2:C:116:DA:N6	2:C:117:DA:N6	0.46	2.64	12	6
1:B:105:DG:OP1	3:A:64:GLU:OE1	0.45	2.35	20	3
3:A:40:ASP:OD2	3:A:40:ASP:N	0.45	2.49	2	4
1:B:102:DT:O2	2:C:128:DA:C2	0.45	2.70	3	2
3:A:59:VAL:O	3:A:63:ARG:CG	0.45	2.64	12	1
2:C:119:DC:C4	2:C:120:DG:O6	0.45	2.69	17	5
2:C:122:DG:C5	2:C:123:DC:N4	0.45	2.85	19	1
3:A:62:TYR:O	3:A:66:LEU:HD12	0.45	2.11	17	3
3:A:70:SER:O	3:A:71:SER:OG	0.45	2.32	8	2
3:A:70:SER:C	3:A:71:SER:OG	0.45	2.55	2	1
1:B:111:DT:C5	1:B:112:DT:H72	0.45	2.47	11	1
3:A:30:GLU:CD	3:A:74:ARG:HH12	0.45	2.15	11	1
3:A:62:TYR:C	3:A:64:GLU:N	0.44	2.70	7	2
3:A:70:SER:OG	3:A:72:ARG:CG	0.44	2.65	8	1
1:B:106:DG:N2	2:C:124:DC:O2	0.44	2.50	11	1
3:A:65:MET:CG	3:A:66:LEU:N	0.44	2.79	1	4
1:B:104:DT:OP2	3:A:40:ASP:OD1	0.44	2.35	15	3
3:A:73:GLU:OE1	3:A:73:GLU:C	0.44	2.55	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:62:TYR:O	3:A:63:ARG:C	0.44	2.56	20	3
3:A:64:GLU:OE2	3:A:64:GLU:O	0.44	2.36	8	1
1:B:106:DG:N2	2:C:124:DC:C2	0.44	2.86	11	1
2:C:127:DA:C2	2:C:128:DA:C5	0.44	3.06	1	3
2:C:121:DT:OP1	3:A:53:LYS:O	0.44	2.36	3	1
1:B:102:DT:C4	1:B:103:DT:C4	0.44	3.05	7	1
2:C:123:DC:H41	3:A:57:ARG:CZ	0.44	2.26	12	1
1:B:104:DT:OP2	3:A:40:ASP:OD2	0.44	2.35	13	3
2:C:119:DC:O3'	3:A:62:TYR:OH	0.43	2.36	18	1
1:B:102:DT:C2	2:C:128:DA:C2	0.43	3.07	18	5
2:C:122:DG:O6	2:C:123:DC:N4	0.43	2.51	3	1
3:A:22:MET:C	3:A:24:LEU:H	0.43	2.16	3	2
3:A:45:ASN:OD1	3:A:45:ASN:C	0.43	2.55	5	1
3:A:21:LEU:HD22	3:A:54:VAL:CG2	0.43	2.43	14	1
2:C:120:DG:P	3:A:58:THR:HG21	0.43	2.53	15	2
1:B:107:DC:N4	3:A:61:LYS:HZ3	0.43	2.12	5	1
3:A:38:TYR:O	3:A:71:SER:OG	0.43	2.32	14	1
1:B:106:DG:O6	2:C:122:DG:O6	0.43	2.37	4	4
1:B:104:DT:C7	3:A:56:ARG:NH1	0.43	2.82	1	1
3:A:24:LEU:CD2	3:A:24:LEU:N	0.43	2.81	8	3
1:B:111:DT:C5	1:B:112:DT:C7	0.42	3.02	7	2
2:C:120:DG:OP1	3:A:62:TYR:OH	0.42	2.34	19	1
3:A:43:ILE:O	3:A:47:LEU:HD13	0.42	2.14	11	3
3:A:22:MET:HG2	3:A:23:LYS:N	0.42	2.29	18	3
1:B:109:DC:N4	2:C:119:DC:H42	0.42	2.11	5	2
1:B:104:DT:OP1	3:A:63:ARG:NH2	0.42	2.52	17	1
3:A:19:GLY:O	3:A:23:LYS:NZ	0.42	2.40	20	1
2:C:122:DG:C8	3:A:57:ARG:NE	0.42	2.86	4	1
1:B:104:DT:H73	3:A:40:ASP:OD2	0.42	2.15	7	1
1:B:106:DG:C6	1:B:107:DC:N4	0.42	2.88	19	1
3:A:23:LYS:O	3:A:27:GLU:CB	0.42	2.67	1	1
1:B:105:DG:OP1	3:A:64:GLU:CD	0.42	2.58	10	4
3:A:43:ILE:HD11	3:A:63:ARG:NH1	0.42	2.30	7	1
3:A:69:PRO:O	3:A:70:SER:OG	0.42	2.37	7	1
1:B:106:DG:C6	3:A:57:ARG:NH2	0.42	2.88	18	1
3:A:40:ASP:OD1	3:A:40:ASP:N	0.42	2.53	5	1
3:A:40:ASP:O	3:A:59:VAL:HG11	0.42	2.15	8	1
3:A:63:ARG:NH1	3:A:63:ARG:CG	0.41	2.81	14	1
3:A:26:LYS:CD	3:A:26:LYS:N	0.41	2.80	8	1
3:A:40:ASP:HA	3:A:43:ILE:HD11	0.41	1.93	10	1
3:A:73:GLU:CD	3:A:73:GLU:C	0.41	2.79	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:116:DA:C2	2:C:117:DA:C2	0.41	3.09	13	1
1:B:104:DT:OP2	3:A:40:ASP:CG	0.41	2.59	3	4
3:A:62:TYR:CD2	3:A:65:MET:SD	0.41	3.14	4	1
3:A:62:TYR:C	3:A:64:GLU:H	0.41	2.17	7	1
2:C:117:DA:H2'	2:C:118:DA:C8	0.41	2.51	12	2
3:A:41:GLN:NE2	3:A:42:GLU:HA	0.41	2.31	15	1
3:A:62:TYR:CD1	3:A:65:MET:SD	0.41	3.14	18	1
3:A:53:LYS:H	3:A:53:LYS:HD2	0.41	1.76	4	1
3:A:57:ARG:O	3:A:61:LYS:CG	0.41	2.69	4	1
3:A:30:GLU:OE2	3:A:34:LYS:NZ	0.41	2.52	8	1
3:A:63:ARG:NH1	3:A:71:SER:OG	0.40	2.53	4	1
3:A:16:LEU:HD12	3:A:21:LEU:CD2	0.40	2.44	8	1
3:A:59:VAL:CG1	3:A:60:ALA:N	0.40	2.82	13	1
1:B:106:DG:O6	1:B:107:DC:N4	0.40	2.54	19	1
3:A:62:TYR:O	3:A:64:GLU:N	0.40	2.55	20	1
3:A:22:MET:O	3:A:66:LEU:CD2	0.40	2.69	14	1
3:A:42:GLU:O	3:A:46:ILE:HD12	0.40	2.16	12	1
2:C:127:DA:C2	2:C:128:DA:C4	0.40	3.09	13	1
2:C:119:DC:C5'	3:A:62:TYR:OH	0.40	2.69	14	1
3:A:16:LEU:HD22	3:A:20:GLU:OE2	0.40	2.15	13	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	59/63 (94%)	45±2 (77±3%)	8±2 (14±3%)	6±1 (10±2%)	1	10
All	All	1180/1260 (94%)	903 (77%)	160 (14%)	117 (10%)	1	10

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	40	ASP	20
3	A	51	GLY	20

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Mol	Chain	Res	Type	Models (Total)
3	A	53	LYS	20
3	A	67	GLY	20
3	A	17	THR	15
3	A	70	SER	10
3	A	69	PRO	4
3	A	16	LEU	2
3	A	66	LEU	2
3	A	19	GLY	2
3	A	71	SER	2

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
3	A	53/57 (93%)	46±1 (87±3%)	7±1 (13±3%)	7 48
All	All	1060/1140 (93%)	920 (87%)	140 (13%)	7 48

All 20 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	59	VAL	20
3	A	43	ILE	18
3	A	53	LYS	18
3	A	26	LYS	14
3	A	31	ASN	14
3	A	66	LEU	14
3	A	63	ARG	9
3	A	25	ILE	6
3	A	71	SER	6
3	A	23	LYS	3
3	A	57	ARG	3
3	A	22	MET	3
3	A	35	ARG	2
3	A	68	ILE	2
3	A	74	ARG	2
3	A	18	GLN	2

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Mol	Chain	Res	Type	Models (Total)
3	A	64	GLU	1
3	A	70	SER	1
3	A	40	ASP	1
3	A	36	LYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

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 monosaccharides 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

No chemical shift data were provided