

Full wwPDB NMR Structure Validation Report (i)

Oct 23, 2021 – 05:43 PM EDT

PDB ID : 1TF3

Title : TFIIIA FINGER 1-3 BOUND TO DNA, NMR, 22 STRUCTURES

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Deposited on : 1997-07-01

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)

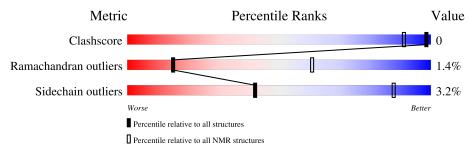
Validation Pipeline (wwPDB-VP) : 2.23.2

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	NMR archive		
Metric	$(\# \mathrm{Entries})$	$(\# \mathrm{Entries})$		
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	Е	15	33%	60%	7%	
2	F	15	33%	60%	7%	
3	A	92		89%	5% 5%	



2 Ensemble composition and analysis (i)

This entry contains 22 models. Model 12 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:13-A:99 (87)	0.41	12		

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 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	3, 7, 13, 14, 16, 19, 21, 22
2	2, 5, 9, 10, 12
3	8, 11, 15
4	4, 6, 17
Single-model clusters	1; 18; 20



3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2412 atoms, of which 1054 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called 5S RNA GENE.

Mol	Chain	Residues	Atoms			Trace			
1	E	15	Total	С	Н	N	О	Р	0
1	E	10	482	148	170	62	88	14	U

• Molecule 2 is a DNA chain called 5S RNA GENE.

Mol	Chain	Residues	Atoms			Trace			
9	E	15	Total	С	Н	N	О	Р	0
	Г	10	467	143	170	52	88	14	U

• Molecule 3 is a protein called TRANSCRIPTION FACTOR IIIA.

Mol	Chain	Residues	Atoms				Trace		
9	Λ	02	Total	С	Н	N	О	S	0
3	A	92	1460	466	714	140	132	8	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	TYR	engineered mutation	UNP P03001
A	35	SER	CYS	engineered mutation	UNP P03001

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms
1	Λ	9	Total Zn
4	A	3	3 3

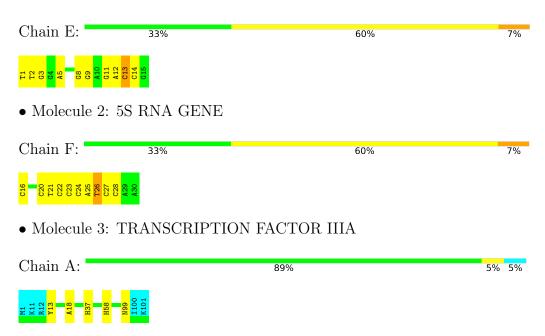


4 Residue-property plots (i)

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.





4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

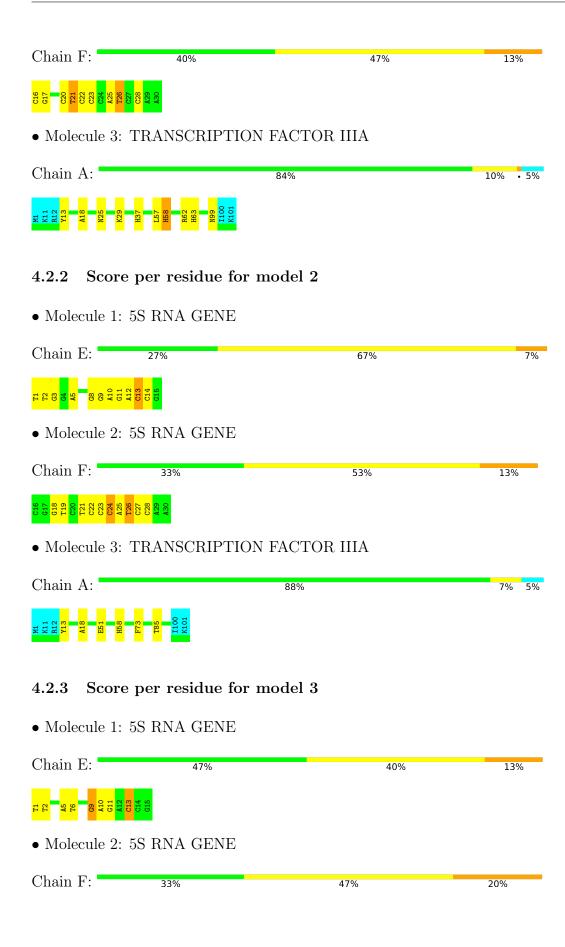
4.2.1 Score per residue for model 1

• Molecule 1: 5S RNA GENE

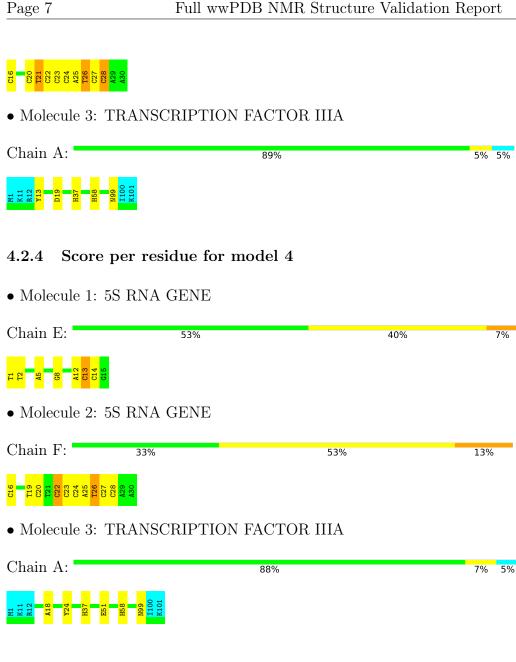


• Molecule 2: 5S RNA GENE



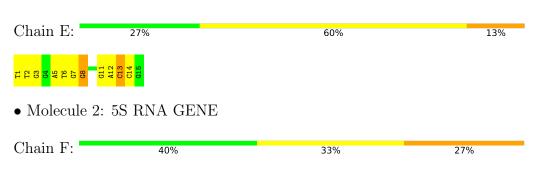






4.2.5Score per residue for model 5

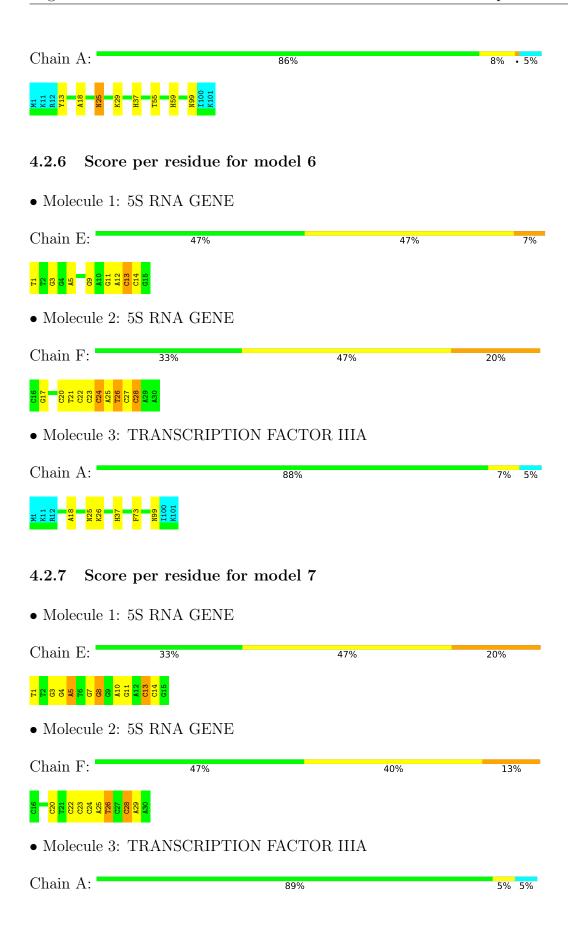
• Molecule 1: 5S RNA GENE





• Molecule 3: TRANSCRIPTION FACTOR IIIA









4.2.8 Score per residue for model 8

• Molecule 1: 5S RNA GENE

Chain E: 33% 60% 7%

T11 T22 G33 G4 A5 G7 G7 A10 G11 A11 C13 G15

• Molecule 2: 5S RNA GENE

Chain F: 40% 40% 20%

C16 T19 C20 C22 C23 C23 C24 A25 T26 C27 C28 A29

• Molecule 3: TRANSCRIPTION FACTOR IIIA

Chain A: 87% 8% 5%



4.2.9 Score per residue for model 9

• Molecule 1: 5S RNA GENE

Chain E: 47% 47% 7%



• Molecule 2: 5S RNA GENE

Chain F: 53% 33% 13%

C16 C20 C23 C23 C24 A25 C24 T26 C24 A25 C24 A25 C24 A25 A26 A30

• Molecule 3: TRANSCRIPTION FACTOR IIIA

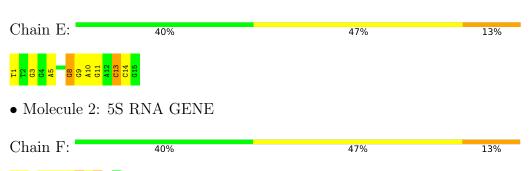
Chain A: 88% 7% 5%





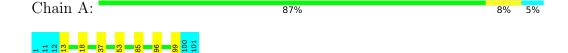
4.2.10 Score per residue for model 10

• Molecule 1: 5S RNA GENE



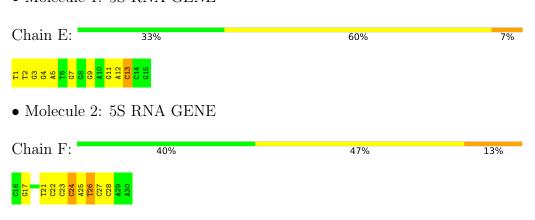


• Molecule 3: TRANSCRIPTION FACTOR IIIA



4.2.11 Score per residue for model 11

• Molecule 1: 5S RNA GENE



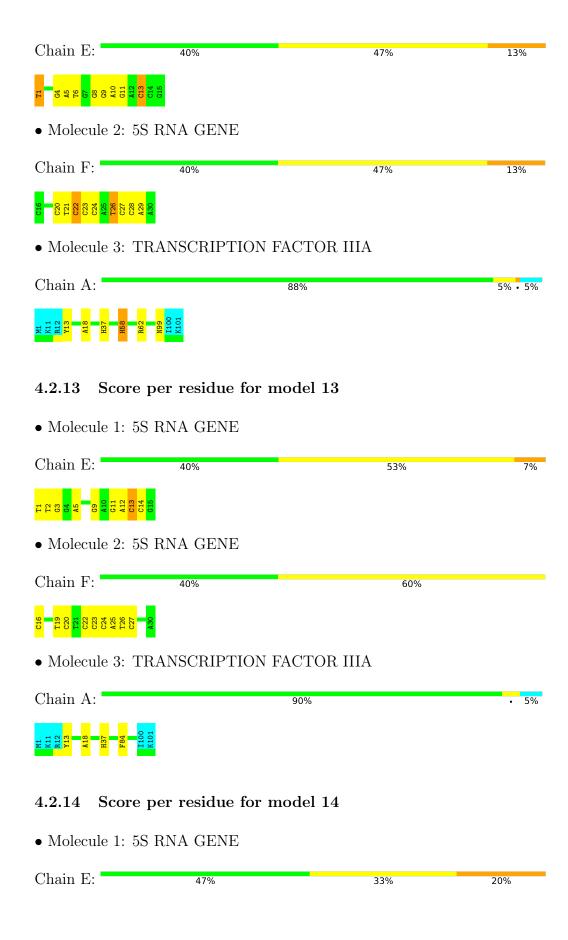
• Molecule 3: TRANSCRIPTION FACTOR IIIA



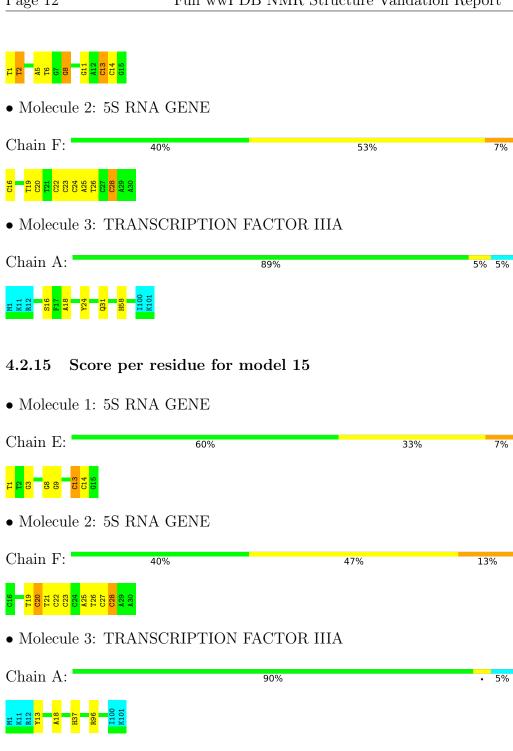
4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: 5S RNA GENE









4.2.16 Score per residue for model 16

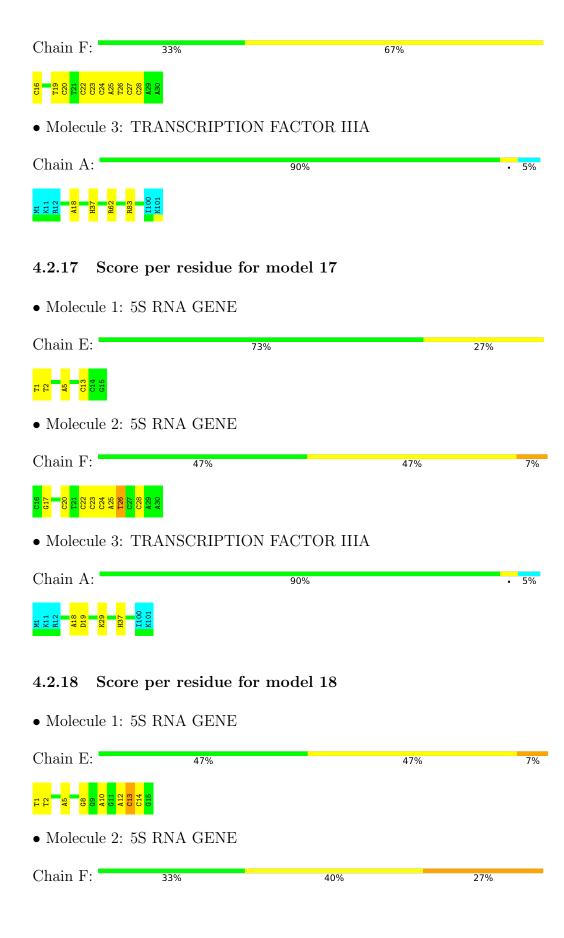
• Molecule 1: 5S RNA GENE

Chain E: 27% 60% 13%

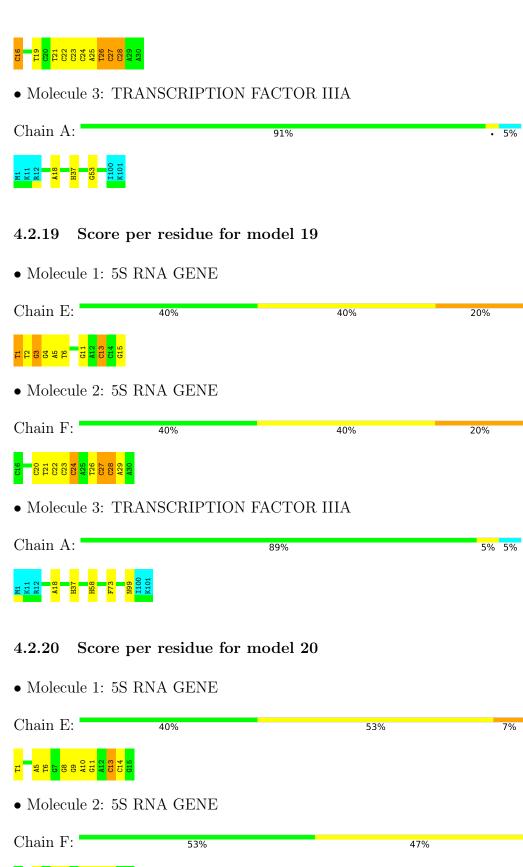
11 12 63 64 A5 16 67 68 69 A10 611 A12 C13

• Molecule 2: 5S RNA GENE





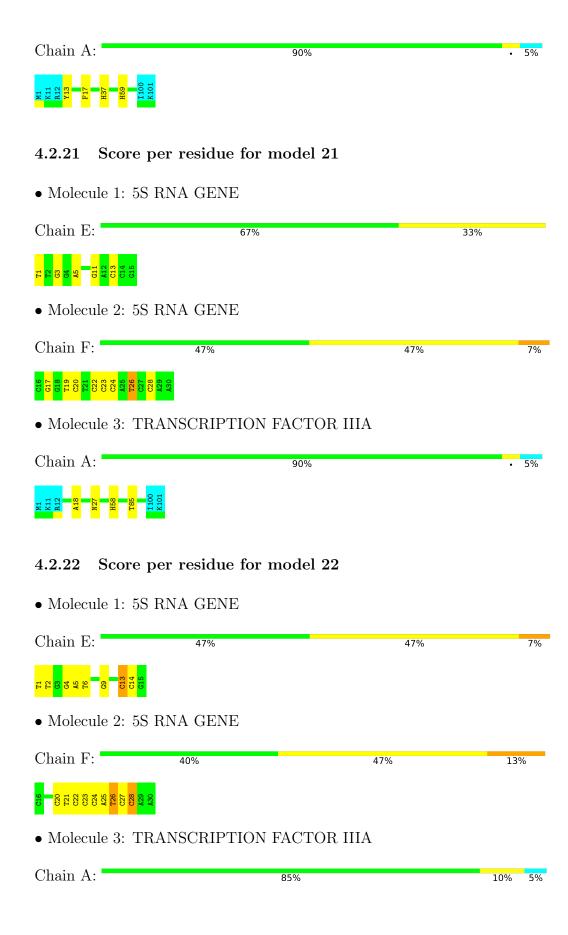




C16
C20
C20
C22
C23
C23
C24
A25
C27
C27
C28
A26
A30

• Molecule 3: TRANSCRIPTION FACTOR IIIA











Refinement protocol and experimental data overview (i) 5



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

Of the 64 calculated structures, 22 were deposited, based on the following criterion: RESTRAINT ENERGIES < 11 KCAL, NO DISTANCE VIOLATIONS > 0.3 A.

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

Software name	Classification	Version
Amber	refinement	
Amber	structure solution	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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).

Mal	Chain	Bond lengths		Bond angles		
Mol Chain		RMSZ	#Z>5	RMSZ	#Z>5	
1	Е	1.20 ± 0.01	$0\pm0/351~(~0.0\pm~0.0\%)$	1.91 ± 0.03	$7\pm1/542~(~1.3\pm~0.3\%)$	
2	F	1.21 ± 0.01	$0\pm0/331~(~0.0\pm~0.0\%)$	1.89 ± 0.03	$8\pm2/507~(~1.7\pm~0.4\%)$	
3	A	0.58 ± 0.00	$0\pm0/722$ ($0.0\pm~0.0\%$)	0.88 ± 0.02	$0\pm0/969~(~0.0\pm~0.0\%)$	
All	All	0.94	0/30888 ($0.0%$)	1.50	337/44396 (0.8%)	

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

Mol	Chain	Chirality	Planarity
1	Е	0.0 ± 0.0	$3.8{\pm}1.6$
2	F	0.0 ± 0.0	$4.3{\pm}1.5$
3	A	0.0 ± 0.0	2.0 ± 0.8
All	All	0	223

There are no bond-length outliers.

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	Atoma	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$	Models	
MIOI	Chain	nes	Type	Atoms		Observed()	ideai()	Worst	Total
2	F	22	DC	O4'-C1'-N1	12.05	116.43	108.00	15	20
1	Е	9	DG	O4'-C1'-N9	9.29	114.50	108.00	11	11
2	F	23	DC	O4'-C1'-N1	9.12	114.39	108.00	4	21
1	Е	8	DG	O4'-C1'-N9	8.05	113.64	108.00	15	12
2	F	20	DC	O4'-C1'-N1	7.84	113.49	108.00	17	19
1	Е	5	DA	O4'-C1'-N9	7.44	113.20	108.00	1	21
1	Е	11	DG	O4'-C1'-N9	7.23	113.06	108.00	10	16
2	F	17	DG	O4'-C1'-N9	6.92	112.85	108.00	6	5

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	Chair				\mathbf{Z}	Observed(0)	Ideal(0)	Mod	dels
Mol	Chain	Res	Type	Atoms		$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$	Worst	Total
1	Е	13	DC	O4'-C1'-N1	6.77	112.74	108.00	7	6
2	F	16	DC	O4'-C1'-N1	6.60	112.62	108.00	8	5
2	F	26	DT	O4'-C1'-N1	6.37	112.46	108.00	6	16
2	F	23	DC	N1-C2-O2	6.20	122.62	118.90	7	8
2	F	22	DC	C1'-O4'-C4'	-6.17	103.93	110.10	15	6
2	F	24	DC	N1-C2-O2	6.13	122.58	118.90	12	19
1	Е	8	DG	O4'-C1'-C2'	-6.03	101.07	105.90	15	4
1	Е	3	DG	O4'-C1'-N9	6.02	112.21	108.00	21	13
1	Е	1	DT	C6-C5-C7	-5.94	119.34	122.90	6	21
2	F	21	DT	C6-C5-C7	-5.93	119.34	122.90	12	10
1	Е	9	DG	O4'-C1'-C2'	-5.92	101.16	105.90	1	4
1	Е	6	DT	C6-C5-C7	-5.91	119.36	122.90	22	9
2	F	22	DC	N1-C2-O2	5.75	122.35	118.90	19	13
2	F	19	DT	O4'-C1'-C2'	-5.66	101.37	105.90	14	5
1	Е	13	DC	N1-C2-O2	5.64	122.28	118.90	14	16
2	F	28	DC	O4'-C1'-N1	5.55	111.89	108.00	7	13
2	F	27	DC	N1-C2-O2	5.46	122.18	118.90	19	4
2	F	19	DT	C6-C5-C7	-5.38	119.67	122.90	8	3
2	F	26	DT	C1'-O4'-C4'	-5.29	104.81	110.10	10	5
1	Е	2	DT	C6-C5-C7	-5.28	119.73	122.90	1	8
2	F	20	DC	C1'-O4'-C4'	-5.28	104.82	110.10	20	3
1	Е	11	DG	C1'-O4'-C4'	-5.26	104.84	110.10	6	2
2	F	16	DC	C1'-O4'-C4'	-5.23	104.87	110.10	10	3
2	F	23	DC	C1'-O4'-C4'	-5.23	104.87	110.10	22	3
2	F	17	DG	C1'-O4'-C4'	-5.22	104.88	110.10	17	2
2	F	26	DT	C6-C5-C7	-5.12	119.83	122.90	6	2
1	Е	2	DT	O4'-C1'-N1	5.09	111.56	108.00	11	1
1	Е	15	DG	O4'-C1'-N9	5.08	111.55	108.00	19	1
2	F	22	DC	N3-C2-O2	-5.07	118.35	121.90	19	1
1	Е	13	DC	O4'-C1'-C2'	-5.05	101.86	105.90	2	2
1	Е	11	DG	O4'-C1'-C2'	-5.03	101.87	105.90	16	2
1	Е	5	DA	O4'-C1'-C2'	-5.02	101.89	105.90	7	1
1	Е	2	DT	C1'-O4'-C4'	-5.01	105.09	110.10	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	F	26	DT	Sidechain	22
1	Е	13	DC	Sidechain	19

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Mol	$\frac{\text{Chain}}{\text{Chain}}$	Res	Type	Group	Models (Total)
2	F	25	DA	Sidechain	18
3	A	37	HIS	Sidechain	18
2	F	28	DC	Sidechain	17
1	Е	14	DC	Sidechain	14
2	F	27	DC	Sidechain	12
1	Е	12	DA	Sidechain	11
3	A	13	TYR	Sidechain	11
1	Е	10	DA	Sidechain	8
2	F	24	DC	Sidechain	7
1	Е	4	DG	Sidechain	6
2	F	16	DC	Sidechain	6
1	Е	8	DG	Sidechain	6
1	Е	2	DT	Sidechain	5
3	A	73	PHE	Sidechain	4
1	Е	7	DG	Sidechain	4
2	F	21	DT	Sidechain	3
2	F	19	DT	Sidechain	3
3	A	24	TYR	Sidechain	3
2	F	29	DA	Sidechain	3
3	A	96	ARG	Sidechain	3
1	Е	11	DG	Sidechain	2
3	A	58	HIS	Sidechain	2
1	Е	9	DG	Sidechain	2
2	F	22	DC	Sidechain	2
3	A	83	ARG	Sidechain	2
1	Е	1	DT	Sidechain	2
1	Е	6	DT	Sidechain	2
2	F	18	DG	Sidechain	1
1	Е	5	DA	Sidechain	1
1	Е	15	DG	Sidechain	1
3	A	84	PHE	Sidechain	1
2	F	20	DC	Sidechain	1
1	Е	3	DG	Sidechain	1

6.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	F	297	170	170	0±0
3	A	701	655	654	0±0
All	All	28886	21890	21868	3

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 0.

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

Atom-1	Atom 2	Clash(Å)	Distance (Å)	Models	
Atom-1	Atom-2	Clash(A)	$\operatorname{Distance}(\operatorname{\AA})$	Worst	Total
3:A:57:LEU:HD13	3:A:58:HIS:N	0.49	2.22	1	1
2:F:22:DC:H41	3:A:58:HIS:CD2	0.44	2.31	4	1
2:F:22:DC:N4	3:A:58:HIS:CE1	0.42	2.88	12	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	Perc	entiles
3	A	87/92 (95%)	77±2 (88±2%)	9±2 (10±2%)	1±0 (1±0%)	15	61
All	All	1914/2024 (95%)	1689 (88%)	198 (10%)	27 (1%)	15	61

All 6 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	18	ALA	19
3	A	19	ASP	3
3	A	53	GLY	2
3	A	25	ASN	1
3	A	17	PHE	1
3	A	27	ASN	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	Analysed Rotameric Outlier		Percentiles
3	A	76/81 (94%)	74±2 (97±2%)	2±2 (3±2%)	42 88
All	All	1672/1782 (94%)	1619 (97%)	53 (3%)	42 88

All 14 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	99	ASN	13
3	A	58	HIS	9
3	A	25	ASN	6
3	A	85	THR	5
3	A	29	LYS	4
3	A	62	ARG	3
3	A	51	GLU	3
3	A	59	HIS	2
3	A	30	LEU	2
3	A	31	GLN	2
3	A	63	HIS	1
3	A	55	THR	1
3	A	26	LYS	1
3	A	16	SER	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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

