wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1CO0
Title	:	NMR STUDY OF TRP REPRESSOR-MTR OPERATOR DNA COMPLEX
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Deposited on	:	1999-05-30

This is a wwPDB NMR Structure Validation Summary 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 (1)) were used in the production of this report:

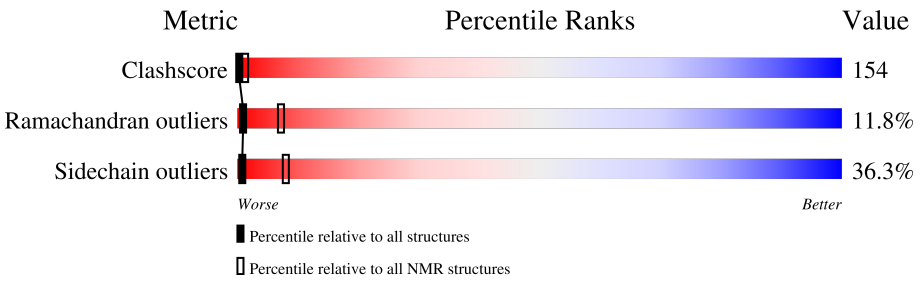
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	E	20	95% 5%
2	F	20	95% 5%
3	A	107	• 57% 23% • 14% •
3	B	107	5% 54% 23% • 15% •

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 4 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:17-A:106, B:18-B:106 (179)	0.79	4

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	4, 7, 10, 11, 12, 14
2	1, 2, 5
3	6, 13, 15
Single-model clusters	3; 8; 9

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4723 atoms, of which 2189 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	E	20	636	196	229	71	121	19	0

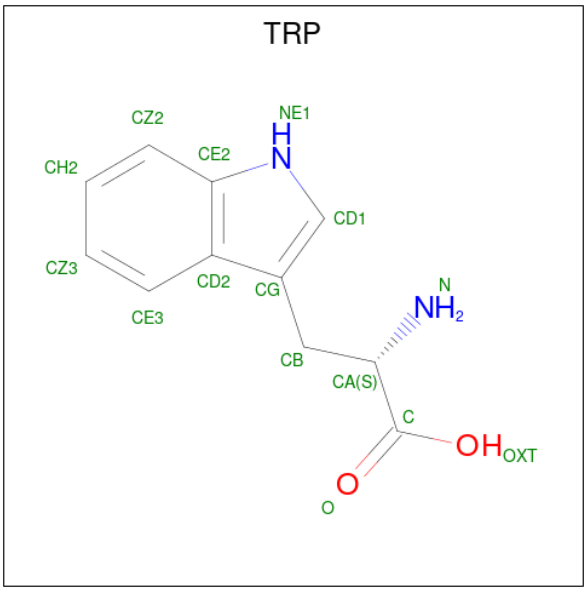
- Molecule 2 is a DNA chain called 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	F	20	633	195	226	78	115	19	0

- Molecule 3 is a protein called TRP OPERON REPRESSOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	A	105	1701	528	856	153	161	3	0
3	B	105	1701	528	856	153	161	3	0

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
4	B	1	26	11	11	2	2
			Total	C	H	N	O
4	B	1	26	11	11	2	2

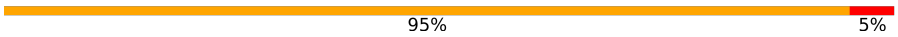
4 Residue-property plots (i)

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.

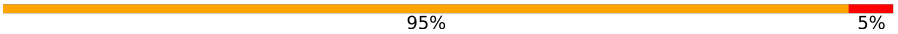
• Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*AP*CP*A)-3'

Chain E:



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

Chain F:

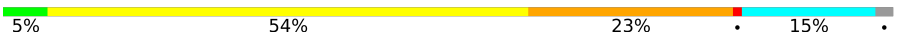


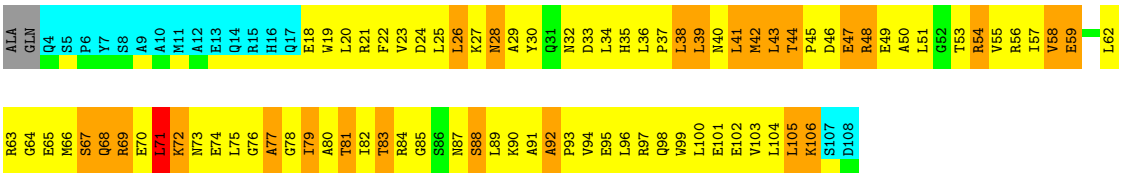
• Molecule 3: TRP OPERON REPRESSOR

Chain A:

• Molecule 3: TRP OPERON REPRESSOR

Chain B:





4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

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

Chain E: 90% 10%

T1 G2 T3 A4 C5 T6 C7 G8 T9 G10 T11 A12 C13 T14 G15 G16 T17 A18 C19 A20

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

Chain F: 10% 80% 10%

T1 G2 T3 A4 C5 C6 A7 G8 T9 A10 C11 A12 C13 G14 A15 G16 T17 A18 C19 A20

• Molecule 3: TRP OPERON REPRESSOR

Chain A: 5% 51% 21% 7% 14% •

ALA GLN Q4 S5 P6 Y7 S8 A9 A10 M11 A12 E13 Q14 R15 H16 Q17 E18 W19 L20 R21 F22 V23 D24 L25 L26 K27 N28 A29 Y30 Q31 N32 D33 L34 H35 L36 P37 L38 L39 N40 L41 M42 L43 T44 P45 D46 E47 R48 E49 A50 L51 G52 T53 R54 V55 R56 I57 V58 E59 E60 L61

L62 R63 G64 E65 M66 S67 Q68 R69 E70 L71 K72 N73 E74 L75 G76 A77 G78 I79 A80 T81 I82 T83 R84 G85 S86 N87 S88 L89 K90 A91 A92 P93 V94 E95 L96 R97 Q98 W99 L100 E101 E102 L105 K106 S107 D108

• Molecule 3: TRP OPERON REPRESSOR

Chain B: 8% 44% 25% 6% 15% •

ALA GLN Q4 S5 P6 Y7 S8 A9 A10 M11 A12 E13 Q14 R15 H16 Q17 E18 W19 L20 R21 F22 V23 D24 L25 L26 K27 N28 A29 Y30 Q31 N32 D33 L34 H35 L36 P37 L38 L39 N40 L41 M42 L43 T44 P45 D46 E47 R48 E49 A50 L51 G52 T53 R54 V55 R56 I57 V58 E59 L62

R63 G64 E65 M66 S67 Q68 R69 E70 L71 K72 N73 G76 A77 G78 I79 A80 T81 I82 T83 R84 G85 S86 N87 S88 L89 K90 A91 A92 P93 V94 E95 L96 R97 Q98 W99 L100 E101 E102 V103 L104 L105 K106 S107 D108

5 Refinement protocol and experimental data overview (i)

Of the 30 calculated structures, 15 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

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	E	2.86±0.01	41±1/455 (9.0± 0.2%)	2.83±0.01	65±2/701 (9.3± 0.3%)
2	F	2.81±0.01	40±0/457 (8.8± 0.0%)	2.84±0.01	64±3/703 (9.1± 0.4%)
3	A	1.09±0.01	0±0/738 (0.0± 0.0%)	1.28±0.01	0±0/998 (0.0± 0.0%)
3	B	1.08±0.00	0±0/729 (0.0± 0.0%)	1.28±0.01	0±0/986 (0.0± 0.0%)
All	All	1.95	1215/35685 (3.4%)	2.07	1942/50820 (3.8%)

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	E	0.0±0.0	0.9±0.7
2	F	0.0±0.0	1.1±0.6
3	A	0.0±0.0	1.1±0.9
3	B	0.0±0.0	0.7±0.7
All	All	0	56

5 of 85 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	F	3	DT	C2'-C1'	-10.60	1.41	1.52	10	15
1	E	12	DA	C2'-C1'	-10.00	1.42	1.52	10	15
1	E	16	DG	C2'-C1'	-9.67	1.42	1.52	4	15
1	E	12	DA	C3'-C2'	-9.67	1.40	1.52	15	15
2	F	13	DC	C3'-C2'	-9.49	1.40	1.52	11	15

5 of 146 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
1	E	12	DA	C3'-C2'-C1'	11.13	115.86	102.50	3	15
1	E	11	DT	C3'-C2'-C1'	11.11	115.83	102.50	11	15
2	F	11	DC	C3'-C2'-C1'	11.01	115.71	102.50	5	15
2	F	12	DA	C3'-C2'-C1'	10.99	115.69	102.50	15	15
2	F	10	DA	C3'-C2'-C1'	10.93	115.61	102.50	11	15

There are no chirality outliers.

5 of 16 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	3	DT	Sidechain	12
1	E	18	DA	Sidechain	10
3	A	56	ARG	Sidechain	6
3	B	54	ARG	Sidechain	6
3	A	54	ARG	Sidechain	4

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	E	407	229	229	78±11
2	F	407	226	226	98±4
3	A	728	755	755	352±18
3	B	719	747	747	287±19
4	B	30	22	18	46±11
All	All	34365	29685	29625	9824

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 154.

5 of 3483 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:43:LEU:C	3:B:45:PRO:HD3	1.43	1.33	6	13
1:E:16:DG:N3	1:E:17:DT:O4	1.32	1.60	3	1
3:A:51:LEU:HD13	3:B:22:PHE:CZ	1.29	1.62	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:72:LYS:HB2	3:A:78:GLY:O	1.24	1.31	13	1
1:E:16:DG:C2	2:F:4:DA:N6	1.23	2.05	3	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	90/107 (84%)	63±4 (70±4%)	17±4 (19±5%)	10±2 (11±2%)	1 8
3	B	89/107 (83%)	54±3 (61±4%)	24±3 (27±4%)	11±3 (13±3%)	1 6
All	All	2685/3210 (84%)	1752 (65%)	615 (23%)	318 (12%)	1 7

5 of 60 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	B	77	ALA	15
3	B	92	ALA	15
3	B	43	LEU	14
3	A	77	ALA	13
3	B	44	THR	13

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	79/92 (86%)	50±3 (64±4%)	29±3 (36±4%)	1 8
3	B	78/92 (85%)	50±4 (64±5%)	28±4 (36±5%)	1 8
All	All	2355/2760 (85%)	1500 (64%)	855 (36%)	1 8

5 of 139 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	41	LEU	15
3	A	58	VAL	15
3	A	90	LYS	15
3	B	72	LYS	15
3	B	90	LYS	15

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	TRP	B	109	-	12,16,16	1.01±0.06	0±0 (0±0%)
4	TRP	B	201	-	12,16,16	1.12±0.16	0±0 (2±3%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	TRP	B	109	-	12,22,22	0.90±0.17	0±1 (1±4%)
4	TRP	B	201	-	12,22,22	1.02±0.14	0±1 (3±5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRP	B	201	-	-	0±0,3,8,8	0±0,2,2,2
4	TRP	B	109	-	-	0±0,3,8,8	0±0,2,2,2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	B	201	TRP	CB-CG	2.74	1.43	1.51	10	5

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
4	B	109	TRP	CB-CG-CD1	3.88	123.17	127.97	8	2
4	B	201	TRP	CB-CG-CD1	3.35	123.82	127.97	8	4
4	B	109	TRP	CB-CG-CD2	2.47	130.09	126.25	8	1
4	B	201	TRP	CB-CG-CD2	2.33	129.88	126.25	2	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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