

wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1WRS
Title	:	NMR STUDY OF HOLO TRP REPRESSOR
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Deposited on	:	1995-05-12

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:

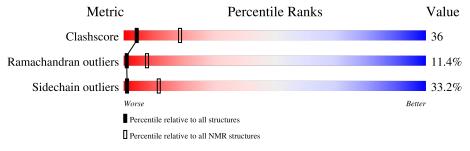
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} {f archive} \ (\# {f Entries})$
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	R	105	17%	40%	14% •	25%	•			
1	S	105	13%	45%	21%	• 18%	•			



2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 2 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	R:15-R:62, R:77-R:106,	0.83	2					
	S:15-S:63, S:72-S:107 (163)							

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 5 single-model clusters were found.

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



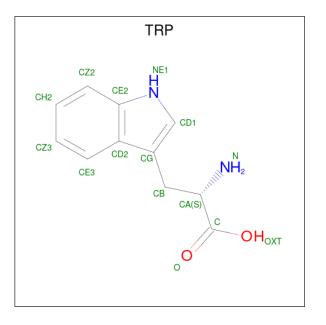
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3432 atoms, of which 1730 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called HOLO TRP REPRESSOR.

Mol	Chain	Residues	Atoms					Trace	
1	D	104	Total	С	Η	Ν	0	S	0
1	1 h		1690	524	854	152	157	3	0
1	C	104	Total	С	Н	Ν	0	S	0
	I S	104	1690	524	854	152	157	3	0

• Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				
0	D	1	Total	С	Η	Ν	0
	n		26	11	11	2	2
0	2 R	1	Total	С	Η	Ν	Ο
			26	11	11	2	2

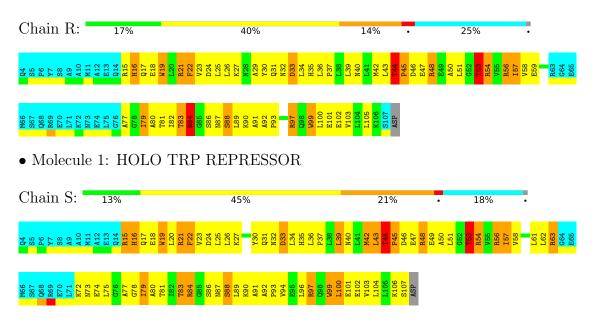


4 Residue-property plots (i)

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.

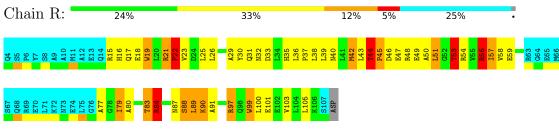
• Molecule 1: HOLO TRP REPRESSOR



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

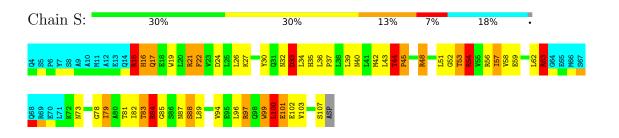
The representative model is number 2. Colouring as in section 4.1 above.

• Molecule 1: HOLO TRP REPRESSOR



• Molecule 1: HOLO TRP REPRESSOR







5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 15 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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		B	ond lengths	Bond angles		
		RMSZ	$\#Z{>}5$	RMSZ	#Z>5	
1	R	1.15 ± 0.01	$4{\pm}0/647$ ($0.6{\pm}$ $0.0\%)$	$1.40{\pm}0.01$	$8{\pm}0/879~(~1.0{\pm}~0.1\%)$	
1	S	$1.17 {\pm} 0.04$	$4{\pm}0/701~(~0.6{\pm}~0.0\%)$	1.41 ± 0.05	$9{\pm}2/948~(~1.0{\pm}~0.2\%)$	
All	All	1.16	121/20220 ($0.6%$)	1.41	265/27405~(~1.0%)	

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	R	$0.0{\pm}0.0$	$6.6 {\pm} 0.5$
1	S	$0.0{\pm}0.0$	7.5 ± 0.5
All	All	0	212

5 of 10 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Mol Chain Res	Chain Res Type	Atoms Z	Observed(Å)	Ideal(Å)	Models			
	Ullaili	nes	туре	Atoms		Observeu(A)	Ideal(A)	Worst	Total
1	R	19	TRP	CG-CD2	-6.57	1.32	1.43	9	15
1	S	99	TRP	CG-CD2	-6.49	1.32	1.43	12	15
1	S	19	TRP	CG-CD2	-6.45	1.32	1.43	12	15
1	R	99	TRP	CG-CD2	-6.14	1.33	1.43	15	15
1	S	76	GLY	N-CA	6.12	1.55	1.46	1	1

5 of 29 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Dec	Type	Atoma	7	Observed(°)	Ideal(°)	Mod	dels
	Unam	nes	Type	Atoms		Observed(*)	Ideal(*)	Worst	Total
1	S	99	TRP	NE1-CE2-CZ2	8.56	139.82	130.40	9	15
1	R	99	TRP	NE1-CE2-CZ2	8.32	139.55	130.40	14	15
1	R	19	TRP	NE1-CE2-CZ2	7.89	139.08	130.40	4	15

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Mol	v	1	10	• .	7	Observed(°)	Ideal(°)	Mod	lels
NIOI	Chain	nes	Type	Atoms	L	Observed(*)	Ideal(*)	Worst	Total
1	S	19	TRP	NE1-CE2-CZ2	7.78	138.96	130.40	15	15
1	R	19	TRP	CD1-NE1-CE2	7.11	115.40	109.00	1	15

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There are no chirality outliers.

5 of 15 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	R	56	ARG	Sidechain	15
1	R	97	ARG	Sidechain	15
1	S	21	ARG	Sidechain	15
1	S	48	ARG	Sidechain	15
1	S	84	ARG	Sidechain	15

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	R	636	662	662	47 ± 10
1	S	691	719	719	$54{\pm}10$
2	R	30	22	21	4 ± 3
All	All	20355	21045	21030	1476

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 36.

5 of 670 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:S:100:LEU:HD22	1:S:101:GLU:H	1.02	1.12	9	2
1:S:100:LEU:HD22	1:S:101:GLU:N	0.97	1.73	14	2
1:R:57:ILE:HD13	1:R:58:VAL:N	0.95	1.77	12	9
1:R:51:LEU:HD23	1:R:52:GLY:N	0.92	1.79	9	1
1:S:57:ILE:HD13	1:S:58:VAL:N	0.91	1.81	10	10



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
1	R	78/105~(74%)	$47 \pm 3 (60 \pm 4\%)$	$23\pm5~(29\pm6\%)$	$9\pm3~(11\pm4\%)$	1 8
1	S	84/105 (80%)	$48\pm3(57\pm4\%)$	$26\pm5(31\pm6\%)$	$10\pm3~(12\pm4\%)$	1 7
All	All	2430/3150~(77%)	1419 (58%)	735 (30%)	276 (11%)	1 8

5 of 76 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	R	44	THR	15
1	R	45	PRO	15
1	S	44	THR	15
1	S	45	PRO	15
1	R	53	THR	14

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	R	69/91~(76%)	$47\pm2~(68\pm3\%)$	22 ± 2 ($32\pm3\%$)	1 12		
1	S	75/91~(82%)	$50\pm2~(66\pm3\%)$	$25\pm2(34\pm3\%)$	1 10		
All	All	2160/2730~(79%)	1443 (67%)	717 (33%)	1 11		

5 of 119 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	R	44	THR	15
1	R	53	THR	15

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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.

Mal	Trune	Chain	Dec	Tinle	Bond lengths			
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	$\#Z{>}2$	
2	TRP	R	1	-	12,16,16	$1.14{\pm}0.07$	$1\pm0~(6\pm3\%)$	
2	TRP	R	109	-	12,16,16	$1.16{\pm}0.09$	1±1 (7±4%)	

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 Chain Res Type Models (Total) R 57ILE 151 1 R 79ILE 151 R 83 THR 15

Mal	Trune	Chain	Dec	Tinle	Bond angles			
INIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	#Z>2	
2	TRP	R	1	-	12,22,22	$1.76 {\pm} 0.12$	4±1 (31±4%)	
2	TRP	R	109	-	12,22,22	$1.77 {\pm} 0.18$	4±0 (30±4%)	

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
2	TRP	R	109	-	-	$0\pm 0,3,8,8$	$0\pm 0,2,2,2$
2	TRP	R	1	-	-	$0\pm 0,3,8,8$	$0\pm0,2,2,2$

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	Ζ	$Observed(\text{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$	Models	
								Worst	Total
2	R	109	TRP	CZ2-CE2	3.23	1.36	1.41	1	12
2	R	1	TRP	CZ2-CE2	2.66	1.37	1.41	1	10
2	R	109	TRP	CE3-CD2	2.25	1.37	1.42	1	2
2	R	1	TRP	CE3-CD2	2.23	1.37	1.42	14	1

5 of 8 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	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathrm{Ideal}(^{o})$	Models	
								Worst	Total
2	R	109	TRP	CB-CG-CD1	4.73	122.12	127.97	13	15
2	R	1	TRP	CB-CG-CD1	3.86	123.20	127.97	12	15
2	R	109	TRP	CZ2-CE2-NE1	3.44	140.31	130.80	15	15
2	R	1	TRP	CZ2-CE2-NE1	3.43	140.29	130.80	14	14
2	R	1	TRP	CD2-CE2-NE1	3.42	100.31	107.92	14	15

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

