



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2021 – 09:24 AM EDT

PDB ID : 7S7V  
Title : Crystal structure of iNicSnFR3a Fluorescent Nicotine Sensor  
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Deposited on : 2021-09-17  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

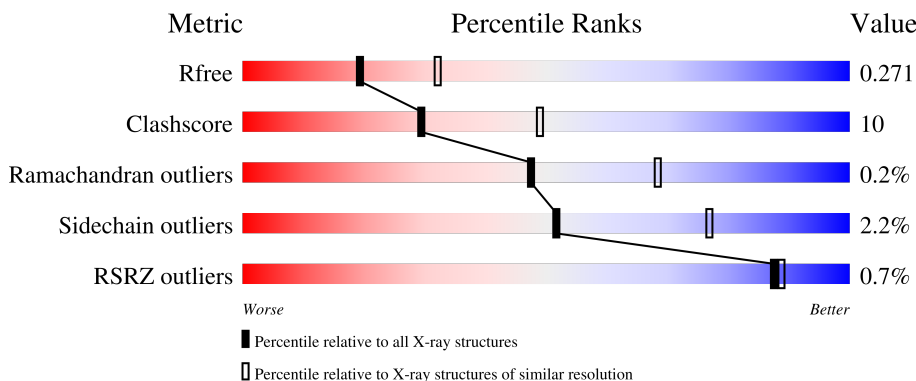
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	537	 72% 22% • 5%
1	B	537	 70% 23% • 5%
1	C	537	 73% 20% • 6%
1	D	537	 74% 20% • 5%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16649 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

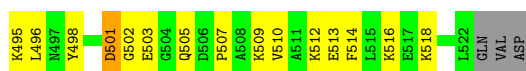
- Molecule 1 is a protein called iNicSnFR 3.0 Fluorescent Nicotine Sensor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4040	2588	671	768	13			
1	B	509	Total	C	N	O	S	0	0	0
			4035	2584	670	768	13			
1	C	507	Total	C	N	O	S	0	0	0
			4024	2578	668	765	13			
1	D	509	Total	C	N	O	S	0	1	0
			4038	2586	670	769	13			

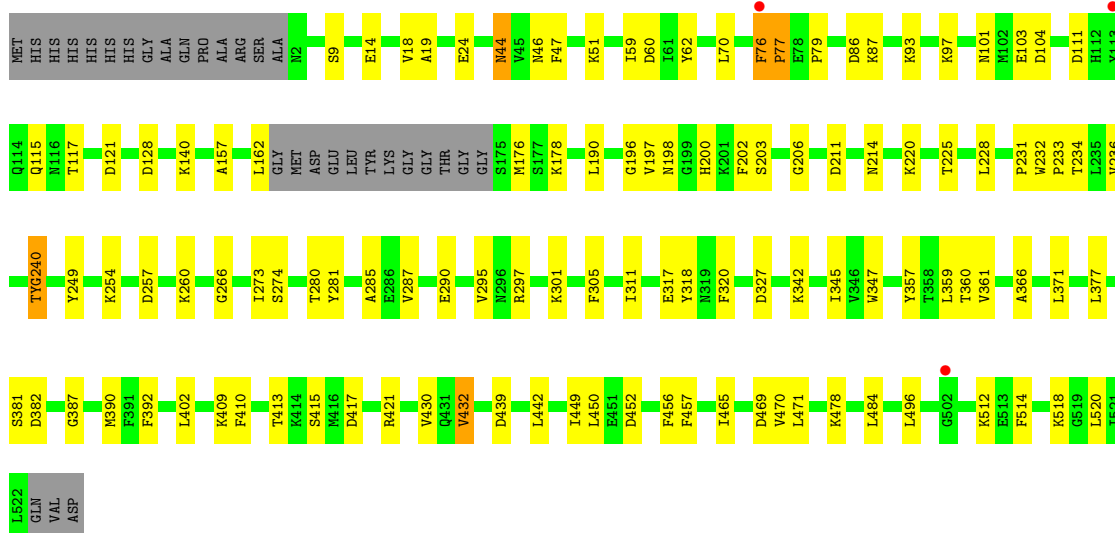
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	134	Total	O	0	0
			134	134		
2	B	112	Total	O	0	0
			112	112		
2	C	147	Total	O	0	0
			147	147		
2	D	119	Total	O	0	0
			119	119		

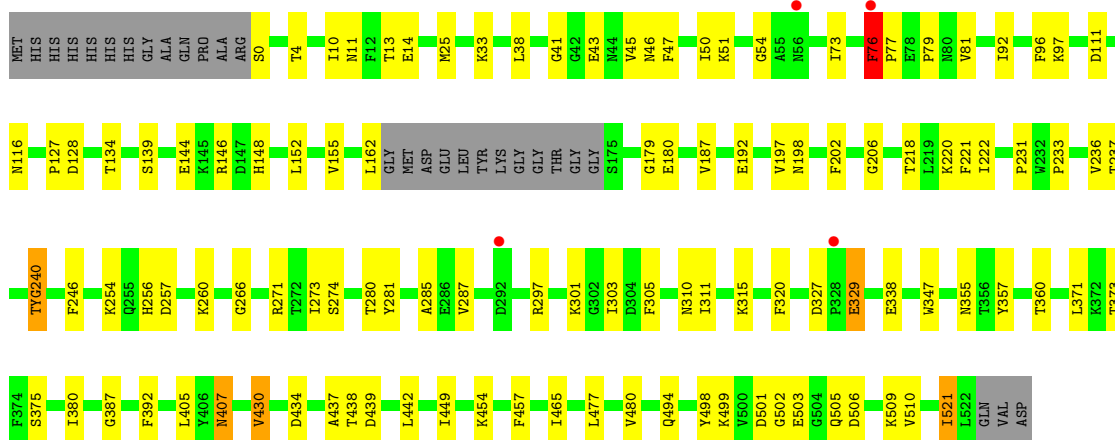
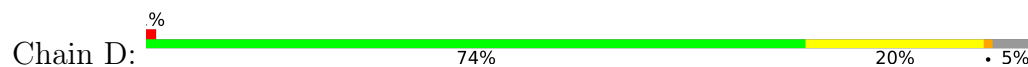




• Molecule 1: iNicSnFR 3.0 Fluorescent Nicotine Sensor



• Molecule 1: iNicSnFR 3.0 Fluorescent Nicotine Sensor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.19Å 86.86Å 91.83Å 75.72° 85.56° 85.28°	Depositor
Resolution (Å)	40.39 – 2.50 45.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.39-2.50) 98.3 (45.47-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.232 , 0.275 0.230 , 0.271	Depositor DCC
$R_{free}$ test set	2007 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 19.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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 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	A	0.31	0/4103	0.53	0/5547
1	B	0.30	0/4098	0.53	0/5540
1	C	0.30	0/4087	0.53	0/5525
1	D	0.31	0/4104	0.55	2/5548 (0.0%)
All	All	0.30	0/16392	0.53	2/22160 (0.0%)

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 outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	327	ASP	CB-CG-OD1	8.30	125.78	118.30
1	D	327	ASP	CB-CG-OD2	-7.97	111.13	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	76	PHE	Peptide
1	B	76	PHE	Peptide
1	C	76	PHE	Peptide
1	D	76	PHE	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4040	0	4022	82	0
1	B	4035	0	4019	87	0
1	C	4024	0	4005	77	0
1	D	4038	0	4024	69	0
2	A	134	0	0	1	0
2	B	112	0	0	6	0
2	C	147	0	0	7	0
2	D	119	0	0	2	0
All	All	16649	0	16070	307	0

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 10.

The worst 5 of 307 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PHE:HE2	1:D:338:GLU:HG3	1.36	0.91
1:B:361:VAL:HG12	1:B:432:VAL:HG12	1.62	0.81
1:A:18:VAL:HG12	1:A:63:VAL:HG21	1.66	0.78
1:A:442:LEU:HD13	1:A:449:ILE:HD11	1.69	0.74
1:C:442:LEU:HD13	1:C:449:ILE:HD11	1.69	0.73

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	502/537 (94%)	492 (98%)	9 (2%)	1 (0%)	47	68
1	B	502/537 (94%)	493 (98%)	8 (2%)	1 (0%)	47	68
1	C	500/537 (93%)	491 (98%)	8 (2%)	1 (0%)	47	68
1	D	503/537 (94%)	492 (98%)	9 (2%)	2 (0%)	34	54
All	All	2007/2148 (93%)	1968 (98%)	34 (2%)	5 (0%)	47	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	PRO
1	D	77	PRO
1	C	77	PRO
1	A	76	PHE
1	D	76	PHE

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
1	A	440/459 (96%)	430 (98%)	10 (2%)	50	76
1	B	439/459 (96%)	426 (97%)	13 (3%)	41	68
1	C	438/459 (95%)	431 (98%)	7 (2%)	62	84
1	D	440/459 (96%)	431 (98%)	9 (2%)	55	79
All	All	1757/1836 (96%)	1718 (98%)	39 (2%)	52	77

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	413	THR
1	D	329	GLU
1	C	432	VAL
1	D	139[A]	SER
1	D	430	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CRO	A	240	1	23,23,24	2.75	8 (34%)	30,32,34	2.60	10 (33%)
1	CRO	B	240	1	23,23,24	2.79	8 (34%)	30,32,34	2.64	8 (26%)
1	CRO	C	240	1	23,23,24	2.79	8 (34%)	30,32,34	2.56	8 (26%)
1	CRO	D	240	1	23,23,24	2.81	8 (34%)	30,32,34	2.55	6 (20%)

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
1	CRO	A	240	1	-	3/12/31/32	0/2/2/2
1	CRO	B	240	1	-	3/12/31/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRO	C	240	1	-	4/12/31/32	0/2/2/2
1	CRO	D	240	1	-	2/12/31/32	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	240	CRO	C1-N2	7.51	1.43	1.32
1	C	240	CRO	C1-N2	7.46	1.43	1.32
1	B	240	CRO	C1-N2	7.42	1.43	1.32
1	A	240	CRO	C1-N2	7.35	1.43	1.32
1	B	240	CRO	CA2-C2	6.15	1.54	1.48

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	CRO	O2-C2-CA2	-7.79	126.58	130.96
1	D	240	CRO	O2-C2-CA2	-7.72	126.63	130.96
1	C	240	CRO	CA2-C2-N3	7.61	106.97	103.37
1	B	240	CRO	CA2-C2-N3	7.30	106.83	103.37
1	D	240	CRO	CA2-C2-N3	7.28	106.81	103.37

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	240	CRO	C3-CA3-N3-C2
1	B	240	CRO	C3-CA3-N3-C2
1	C	240	CRO	C3-CA3-N3-C2
1	D	240	CRO	C3-CA3-N3-C2
1	C	240	CRO	C2-CA2-CB2-CG2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	240	CRO	2	0
1	B	240	CRO	1	0
1	C	240	CRO	1	0
1	D	240	CRO	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	508/537 (94%)	-0.02	5 (0%) 82 84	20, 36, 55, 80	0
1	B	508/537 (94%)	0.09	3 (0%) 89 90	22, 40, 63, 76	0
1	C	506/537 (94%)	-0.02	3 (0%) 89 90	23, 36, 56, 71	0
1	D	508/537 (94%)	0.14	4 (0%) 86 87	25, 41, 63, 103	0
All	All	2030/2148 (94%)	0.05	15 (0%) 87 89	20, 38, 60, 103	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	PHE	3.2
1	D	328	PRO	3.2
1	C	76	PHE	2.8
1	A	109	LEU	2.5
1	B	325	SER	2.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRO	B	240	22/23	0.93	0.18	23,31,36,41	0
1	CRO	D	240	22/23	0.94	0.15	31,35,40,42	0
1	CRO	C	240	22/23	0.95	0.16	22,27,34,36	0
1	CRO	A	240	22/23	0.95	0.14	19,26,32,34	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.