



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 8, 2025 – 10:10 AM EST

PDB ID : 9N7G / pdb\_00009n7g  
Title : Crystal structure of S1007A in complex with FN3  
Authors : Guo, Z.; Alexandrov, K.; Mutschler, R.; Caputo, A.; Cui, Z.  
Deposited on : 2025-02-05  
Resolution : 2.33 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.47

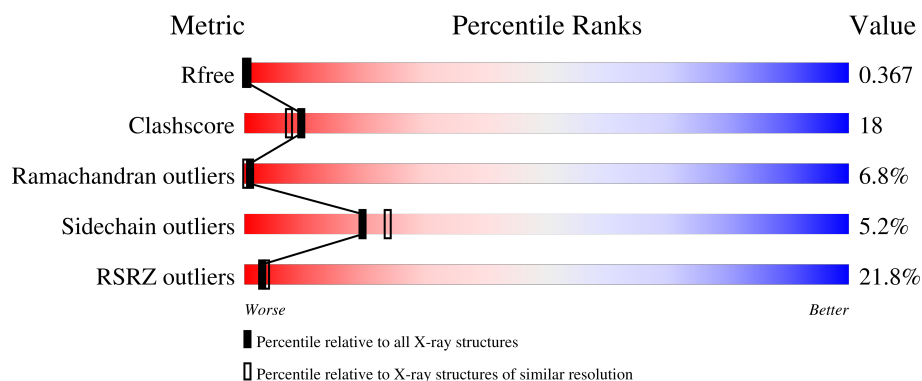
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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))
$R_{free}$	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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	242	
1	B	242	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2795 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 Protein S100-A7 FN3 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	6	0
			1377	867	227	276	7			
1	B	182	Total	C	N	O	S	0	1	0
			1411	892	235	278	6			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLY	-	linker	PDB ?
A	91	GLY	-	linker	PDB ?
A	92	GLY	-	linker	PDB ?
A	93	SER	-	linker	PDB ?
A	94	GLY	-	linker	PDB ?
A	95	GLY	-	linker	PDB ?
A	96	SER	-	linker	PDB ?
A	97	GLY	-	linker	PDB ?
A	98	GLY	-	linker	PDB ?
A	99	ASP	-	linker	PDB ?
A	100	GLY	-	linker	PDB ?
A	101	GLY	-	linker	PDB ?
A	102	GLY	-	linker	PDB ?
A	103	SER	-	linker	PDB ?
A	104	GLY	-	linker	PDB ?
A	105	ASP	-	linker	PDB ?
A	106	GLY	-	linker	PDB ?
A	107	GLY	-	linker	PDB ?
A	108	SER	-	linker	PDB ?
A	109	GLY	-	linker	PDB ?
A	110	SER	-	linker	PDB ?
A	111	GLY	-	linker	PDB ?
A	112	SER	-	linker	PDB ?
A	113	GLY	-	linker	PDB ?
A	114	GLY	-	linker	PDB ?

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLY	-	linker	PDB ?
A	116	GLY	-	linker	PDB ?
A	117	ASP	-	linker	PDB ?
A	118	SER	-	linker	PDB ?
A	119	GLY	-	linker	PDB ?
A	120	SER	-	linker	PDB ?
A	121	SER	-	linker	PDB ?
A	122	GLY	-	linker	PDB ?
A	123	GLY	-	linker	PDB ?
A	124	SER	-	linker	PDB ?
A	125	GLY	-	linker	PDB ?
A	126	SER	-	linker	PDB ?
A	127	GLY	-	linker	PDB ?
A	128	GLY	-	linker	PDB ?
A	129	GLY	-	linker	PDB ?
A	156	ASP	GLU	conflict	UNP P31151
A	230	LYS	-	expression tag	UNP P31151
A	231	LEU	-	expression tag	UNP P31151
A	232	ALA	-	expression tag	UNP P31151
A	233	ALA	-	expression tag	UNP P31151
A	234	ALA	-	expression tag	UNP P31151
A	235	LEU	-	expression tag	UNP P31151
A	236	GLU	-	expression tag	UNP P31151
A	237	HIS	-	expression tag	UNP P31151
A	238	HIS	-	expression tag	UNP P31151
A	239	HIS	-	expression tag	UNP P31151
A	240	HIS	-	expression tag	UNP P31151
A	241	HIS	-	expression tag	UNP P31151
A	242	HIS	-	expression tag	UNP P31151
B	90	GLY	-	linker	PDB ?
B	91	GLY	-	linker	PDB ?
B	92	GLY	-	linker	PDB ?
B	93	SER	-	linker	PDB ?
B	94	GLY	-	linker	PDB ?
B	95	GLY	-	linker	PDB ?
B	96	SER	-	linker	PDB ?
B	97	GLY	-	linker	PDB ?
B	98	GLY	-	linker	PDB ?
B	99	ASP	-	linker	PDB ?
B	100	GLY	-	linker	PDB ?
B	101	GLY	-	linker	PDB ?
B	102	GLY	-	linker	PDB ?

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	SER	-	linker	PDB ?
B	104	GLY	-	linker	PDB ?
B	105	ASP	-	linker	PDB ?
B	106	GLY	-	linker	PDB ?
B	107	GLY	-	linker	PDB ?
B	108	SER	-	linker	PDB ?
B	109	GLY	-	linker	PDB ?
B	110	SER	-	linker	PDB ?
B	111	GLY	-	linker	PDB ?
B	112	SER	-	linker	PDB ?
B	113	GLY	-	linker	PDB ?
B	114	GLY	-	linker	PDB ?
B	115	GLY	-	linker	PDB ?
B	116	GLY	-	linker	PDB ?
B	117	ASP	-	linker	PDB ?
B	118	SER	-	linker	PDB ?
B	119	GLY	-	linker	PDB ?
B	120	SER	-	linker	PDB ?
B	121	SER	-	linker	PDB ?
B	122	GLY	-	linker	PDB ?
B	123	GLY	-	linker	PDB ?
B	124	SER	-	linker	PDB ?
B	125	GLY	-	linker	PDB ?
B	126	SER	-	linker	PDB ?
B	127	GLY	-	linker	PDB ?
B	128	GLY	-	linker	PDB ?
B	129	GLY	-	linker	PDB ?
B	156	ASP	GLU	conflict	UNP P31151
B	230	LYS	-	expression tag	UNP P31151
B	231	LEU	-	expression tag	UNP P31151
B	232	ALA	-	expression tag	UNP P31151
B	233	ALA	-	expression tag	UNP P31151
B	234	ALA	-	expression tag	UNP P31151
B	235	LEU	-	expression tag	UNP P31151
B	236	GLU	-	expression tag	UNP P31151
B	237	HIS	-	expression tag	UNP P31151
B	238	HIS	-	expression tag	UNP P31151
B	239	HIS	-	expression tag	UNP P31151
B	240	HIS	-	expression tag	UNP P31151
B	241	HIS	-	expression tag	UNP P31151
B	242	HIS	-	expression tag	UNP P31151

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	O 4	0	0
2	B	3	Total 3	O 3	0	0



- Molecule 1: Protein S100-A7 FN3 chimera



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.82Å 60.09Å 121.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.67 – 2.33 45.67 – 2.33	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.67-2.33) 45.8 (45.67-2.33)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.271 , 0.367 0.272 , 0.367	Depositor DCC
$R_{free}$ test set	329 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	2795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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](#)

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	0.60	0/1431	1.04	1/1936 (0.1%)
1	B	0.57	0/1446	1.03	3/1957 (0.2%)
All	All	0.59	0/2877	1.04	4/3893 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	LEU	N-CA-C	8.52	123.88	112.30
1	A	153	ASP	CA-CB-CG	6.06	118.66	112.60
1	B	51	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	59	THR	CA-CB-OG1	-5.21	101.79	109.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	1377	0	1286	40	0
1	B	1411	0	1335	65	0
2	A	4	0	0	0	0
2	B	3	0	0	1	0
All	All	2795	0	2621	94	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 18.

The worst 5 of 94 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:B:30:LEU:HD12	1:B:147:LYS:HG2	1.41	1.01
1:B:30:LEU:HD23	1:B:33:TYR:HB3	1.51	0.90
1:B:33:TYR:CE2	1:B:49:VAL:HG21	2.10	0.87
1:B:175:CYS:HG	1:B:224:CYS:HG	1.04	0.83
1:A:219:HIS:CD2	1:B:77:ALA:HB2	2.14	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 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	182/242 (75%)	146 (80%)	21 (12%)	15 (8%)	1	0
1	B	179/242 (74%)	149 (83%)	21 (12%)	9 (5%)	1	0
All	All	361/484 (75%)	295 (82%)	42 (12%)	24 (7%)	1	0

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	26	GLU
1	A	31	HIS
1	A	78	LEU
1	B	76	GLY

### 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	146/188 (78%)	138 (94%)	8 (6%)	18	21
1	B	149/188 (79%)	142 (95%)	7 (5%)	22	28
All	All	295/376 (78%)	280 (95%)	15 (5%)	19	24

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	CYS
1	B	89	THR
1	B	30	LEU
1	B	162	THR
1	B	49	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	181	ASN
1	A	219	HIS
1	B	193	ASN
1	B	219	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	180/242 (74%)	1.42	34 (18%) <b>4</b> <b>5</b>	7, 47, 74, 114	8 (4%)
1	B	182/242 (75%)	1.92	45 (24%) <b>2</b> <b>2</b>	8, 52, 80, 100	6 (3%)
All	All	362/484 (74%)	1.67	79 (21%) <b>3</b> <b>3</b>	7, 49, 77, 114	14 (3%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	VAL	27.4
1	A	24	TRP	26.2
1	B	27	ILE	22.8
1	B	25	PRO	22.7
1	A	25	PRO	22.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.