



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 12:04 PM EST

PDB ID : 1G8T  
Title : SM ENDONUCLEASE FROM SERATIA MARCENSSENS AT 1.1 Å RESOLUTION  
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Deposited on : 2000-11-21  
Resolution : 1.10 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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

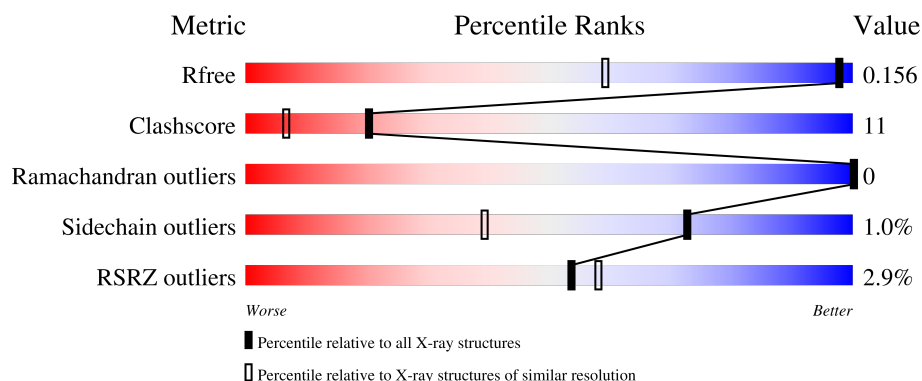
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.10 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	1365 (1.12-1.08)
Clashscore	180529	1561 (1.12-1.08)
Ramachandran outliers	177936	1524 (1.12-1.08)
Sidechain outliers	177891	1520 (1.12-1.08)
RSRZ outliers	164620	1365 (1.12-1.08)

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	245	
1	B	245	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	801	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4736 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 NUCLEASE SM2 ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	25	0
			1934	1210	345	372	7			
1	B	241	Total	C	N	O	S	0	27	0
			1931	1211	343	370	7			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0

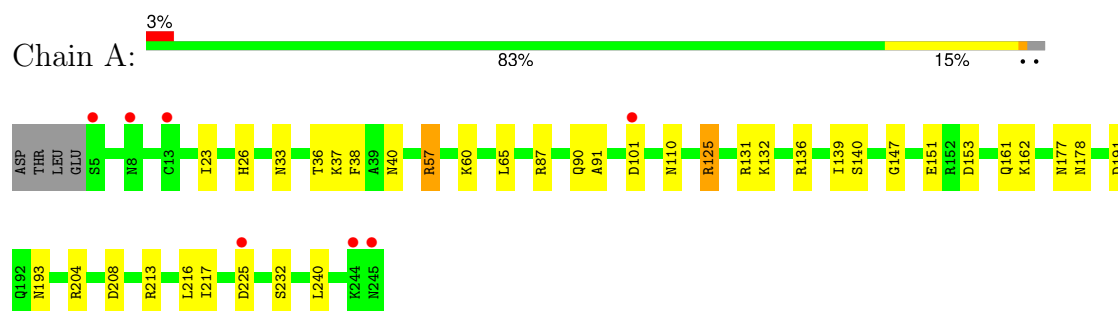
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	440	Total 440	O 440	0	0
4	B	409	Total 409	O 409	0	0

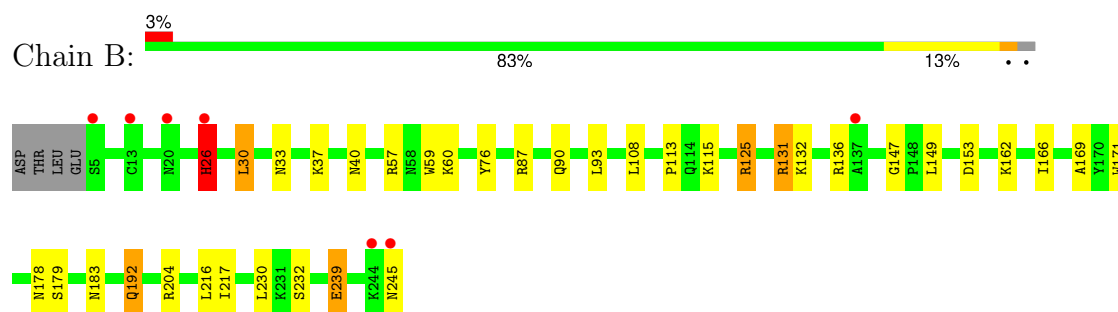
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: NUCLEASE SM2 ISOFORM



#### • Molecule 1: NUCLEASE SM2 ISOFORM



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.39Å 73.67Å 68.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10 20.00 – 1.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (20.00-1.10) 91.5 (20.00-1.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 1.10Å)	Xtriage
Refinement program	REFMAC 4.0.2	Depositor
R, $R_{free}$	0.129 , 0.156 0.133 , 0.156	Depositor DCC
$R_{free}$ test set	9975 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4113e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG

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	0.61	0/2103	1.14	12/2856 (0.4%)
1	B	0.62	0/2121	1.12	16/2878 (0.6%)
All	All	0.61	0/4224	1.13	28/5734 (0.5%)

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

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30[A]	LEU	CA-CB-CG	10.49	139.44	115.30
1	B	30[B]	LEU	CA-CB-CG	10.49	139.44	115.30
1	A	57[A]	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	A	57[B]	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	A	101	ASP	CB-CG-OD2	-8.74	110.44	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151[B]	GLU	Mainchain

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## 5.2 Torsion angles

### 5.2.1 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	264/245 (108%)	250 (95%)	14 (5%)	0	100	100
1	B	266/245 (109%)	256 (96%)	10 (4%)	0	100	100
All	All	530/490 (108%)	506 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.2.2 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	222/203 (109%)	222 (100%)	0	100	100
1	B	225/203 (111%)	219 (97%)	6 (3%)	40	6
All	All	447/406 (110%)	441 (99%)	6 (1%)	73	28

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	GLN
1	B	239[A]	GLU
1	B	239[B]	GLU
1	B	30[A]	LEU
1	B	26	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	40	ASN
1	B	90	GLN
1	B	192	GLN
1	B	120	GLN
1	A	106	ASN

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.4 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.5 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
2	SO4	A	804	-	4,4,4	0.66	0	6,6,6	0.34	0
2	SO4	B	803	-	4,4,4	0.82	0	6,6,6	0.67	0
2	SO4	A	801	-	4,4,4	0.80	0	6,6,6	0.55	0
2	SO4	B	802	-	4,4,4	0.67	0	6,6,6	0.29	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	SO4	1	0
2	A	801	SO4	4	0
2	B	802	SO4	1	0

## 5.6 Other polymers [i](#)

There are no such residues in this entry.

## 5.7 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	241/245 (98%)	-0.28	7 (2%) 54 58	5, 10, 18, 34	24 (9%)
1	B	241/245 (98%)	-0.30	7 (2%) 54 58	6, 10, 18, 39	26 (10%)
All	All	482/490 (98%)	-0.29	14 (2%) 54 58	5, 10, 18, 39	50 (10%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	ASN	5.9
1	A	5	SER	5.7
1	B	26	HIS	5.3
1	B	5	SER	3.5
1	A	245	ASN	3.5

### 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 monosaccharides in this entry.

### 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	804	5/5	0.80	0.14	23,23,24,24	5
2	SO4	B	803	5/5	0.87	0.24	10,10,12,13	5
2	SO4	A	801	5/5	0.90	0.12	18,20,20,21	5
2	SO4	B	802	5/5	0.95	0.09	12,13,16,16	5
3	MG	A	810	1/1	0.99	0.29	7,7,7,7	0
3	MG	B	811	1/1	0.99	0.25	4,4,4,4	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.