Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 05:48 AM EDT

PDB ID	:	1G8T
Title	:	SM ENDONUCLEASE FROM SERATIA MARCENSCENS AT 1.1 A RESOLUTION
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Deposited on	:	2000-11-21
Resolution	:	1.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

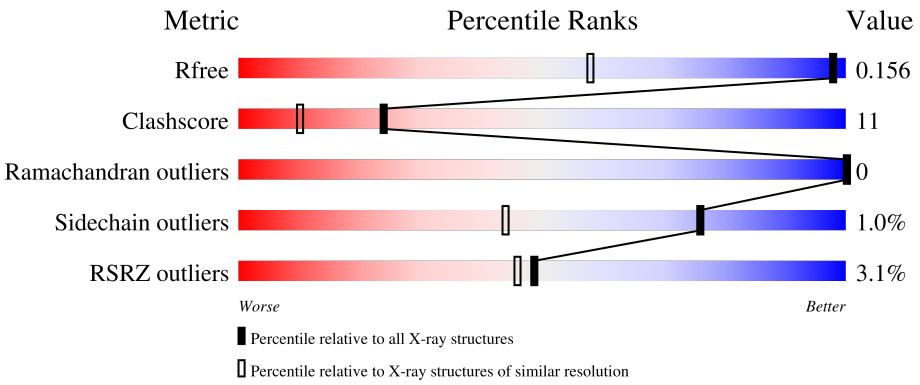
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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}	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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 >=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 <=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	3% 83% 15% • •
1	B	245	3% 83% 13% • •

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)

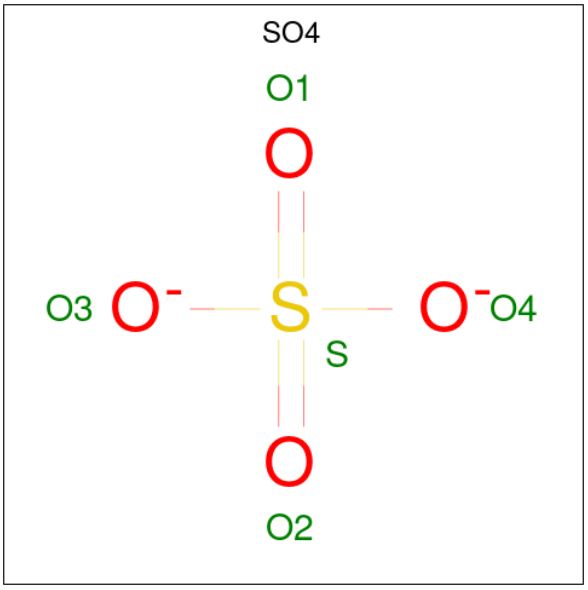
There are 4 unique types of molecules in this entry. The entry contains 4736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	241	1934	1210	345	372	7	0	25	0
1	B	241	1931	1211	343	370	7	0	27	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

- Molecule 4 is water.

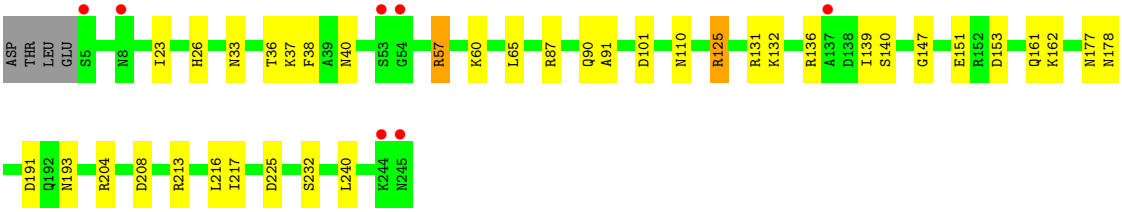
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	440	440	440	0	0
			Total	O		
4	B	409	409	409	0	0

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.

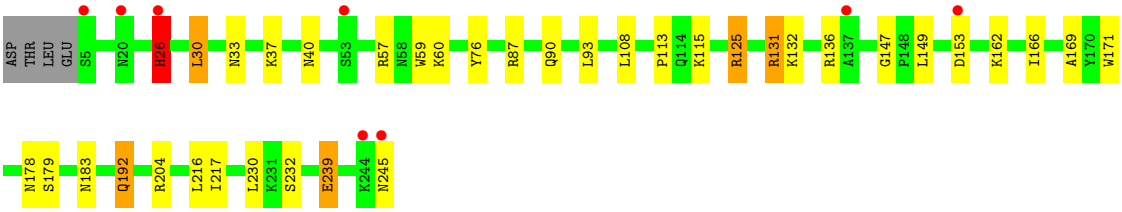
- Molecule 1: NUCLEASE SM2 ISOFORM

Chain A:



- Molecule 1: NUCLEASE SM2 ISOFORM

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.39Å 73.67Å 68.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10 19.92 – 1.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (20.00-1.10) 91.5 (19.92-1.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	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^2)	9.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SO4

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.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	B	26	HIS	ND1-CG-CD2	-8.68	93.84	106.00
1	B	153[A]	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	153[B]	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	136	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	213	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	125[A]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	125[B]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	204[A]	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	204[B]	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ASP	CB-CG-OD1	6.31	123.97	118.30
1	A	87	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	26	HIS	CG-CD2-NE2	6.12	120.84	109.20
1	B	87	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	136	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	B	125[A]	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	125[B]	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	191	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	B	136	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	B	131[A]	ARG	CD-NE-CZ	-5.31	116.17	123.60
1	B	131[B]	ARG	CD-NE-CZ	-5.31	116.17	123.60
1	B	136	ARG	O-C-N	-5.08	114.58	122.70
1	B	26	HIS	CB-CG-ND1	5.04	135.81	123.20
1	A	225	ASP	CB-CG-OD1	-5.04	113.77	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

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles (i)

5.2.1 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	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 (i)

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%)	44 9
All	All	447/406 (110%)	441 (99%)	6 (1%)	76 32

All (6) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	40	ASN
1	A	90	GLN
1	A	106	ASN
1	A	110	ASN
1	A	177	ASN
1	B	8	ASN
1	B	40	ASN
1	B	90	GLN
1	B	120	GLN
1	B	183	ASN
1	B	192	GLN

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 monosaccharides 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	801	1	4,4,4	0.73	0	6,6,6	0.60	0
2	SO4	B	802	1	4,4,4	0.60	0	6,6,6	0.27	0
2	SO4	B	803	-	4,4,4	0.76	0	6,6,6	0.70	0
2	SO4	A	804	-	4,4,4	0.58	0	6,6,6	0.34	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	801	SO4	4	0
2	B	802	SO4	1	0
2	A	804	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, 95th 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^2)	Q<0.9
1	A	241/245 (98%)	-0.31	7 (2%)	51	49	6, 10, 18, 34	0
1	B	241/245 (98%)	-0.32	8 (3%)	46	43	7, 10, 19, 39	0
All	All	482/490 (98%)	-0.31	15 (3%)	49	46	6, 10, 19, 39	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	SER	8.4
1	B	245	ASN	6.3
1	B	5	SER	5.6
1	B	137	ALA	4.4
1	A	245	ASN	4.1
1	A	137	ALA	3.9
1	B	26	HIS	3.0
1	B	244	LYS	2.6
1	B	20	ASN	2.6
1	A	244	LYS	2.5
1	A	8	ASN	2.4
1	A	53	SER	2.4
1	A	54	GLY	2.3
1	B	53[A]	SER	2.2
1	B	153[A]	ASP	2.0

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, 95th 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^2)	Q<0.9
2	SO4	B	803	5/5	0.91	0.34	10,10,12,13	5
2	SO4	A	801	5/5	0.92	0.17	18,20,20,21	5
2	SO4	A	804	5/5	0.93	0.17	23,23,24,24	5
2	SO4	B	802	5/5	0.96	0.13	12,13,16,16	5
3	MG	A	810	1/1	0.99	0.23	7,7,7,7	0
3	MG	B	811	1/1	0.99	0.19	4,4,4,4	0

6.5 Other polymers (i)

There are no such residues in this entry.