



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:16 AM BST

PDB ID : 6S58
Title : AvaII restriction endonuclease in the absence of nucleic acids
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Deposited on : 2019-06-30
Resolution : 2.32 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

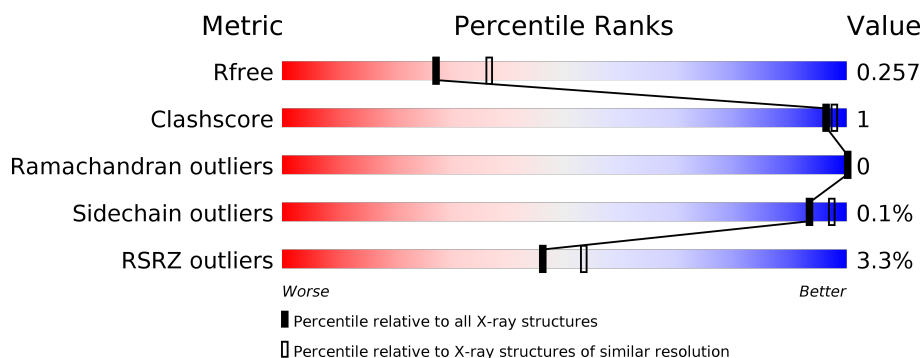
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 on 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 $\leq 5\%$. 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	238	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div></div> </div>
1	B	238	<div> <div>%</div> <div> <div></div> <div>88%</div> <div></div> </div> <div>10%</div> </div>
1	C	238	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div></div> </div>
1	D	238	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div></div> </div> <div>6%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	A	303	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7364 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 Type II site-specific deoxyribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1874	1191	324	353	6			
1	B	215	Total	C	N	O	S	0	0	0
			1727	1097	293	331	6			
1	C	233	Total	C	N	O	S	0	1	0
			1879	1194	324	355	6			
1	D	223	Total	C	N	O	S	0	0	0
			1781	1134	301	340	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8YYB7
A	2	GLY	-	expression tag	UNP Q8YYB7
A	231	LEU	-	expression tag	UNP Q8YYB7
A	232	GLU	-	expression tag	UNP Q8YYB7
A	233	HIS	-	expression tag	UNP Q8YYB7
A	234	HIS	-	expression tag	UNP Q8YYB7
A	235	HIS	-	expression tag	UNP Q8YYB7
A	236	HIS	-	expression tag	UNP Q8YYB7
A	237	HIS	-	expression tag	UNP Q8YYB7
A	238	HIS	-	expression tag	UNP Q8YYB7
B	1	MET	-	initiating methionine	UNP Q8YYB7
B	2	GLY	-	expression tag	UNP Q8YYB7
B	231	LEU	-	expression tag	UNP Q8YYB7
B	232	GLU	-	expression tag	UNP Q8YYB7
B	233	HIS	-	expression tag	UNP Q8YYB7
B	234	HIS	-	expression tag	UNP Q8YYB7
B	235	HIS	-	expression tag	UNP Q8YYB7
B	236	HIS	-	expression tag	UNP Q8YYB7
B	237	HIS	-	expression tag	UNP Q8YYB7
B	238	HIS	-	expression tag	UNP Q8YYB7
C	1	MET	-	initiating methionine	UNP Q8YYB7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	GLY	-	expression tag	UNP Q8YYB7
C	231	LEU	-	expression tag	UNP Q8YYB7
C	232	GLU	-	expression tag	UNP Q8YYB7
C	233	HIS	-	expression tag	UNP Q8YYB7
C	234	HIS	-	expression tag	UNP Q8YYB7
C	235	HIS	-	expression tag	UNP Q8YYB7
C	236	HIS	-	expression tag	UNP Q8YYB7
C	237	HIS	-	expression tag	UNP Q8YYB7
C	238	HIS	-	expression tag	UNP Q8YYB7
D	1	MET	-	initiating methionine	UNP Q8YYB7
D	2	GLY	-	expression tag	UNP Q8YYB7
D	231	LEU	-	expression tag	UNP Q8YYB7
D	232	GLU	-	expression tag	UNP Q8YYB7
D	233	HIS	-	expression tag	UNP Q8YYB7
D	234	HIS	-	expression tag	UNP Q8YYB7
D	235	HIS	-	expression tag	UNP Q8YYB7
D	236	HIS	-	expression tag	UNP Q8YYB7
D	237	HIS	-	expression tag	UNP Q8YYB7
D	238	HIS	-	expression tag	UNP Q8YYB7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total X 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	38	Total O 38 38	0	0

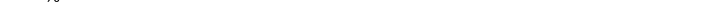
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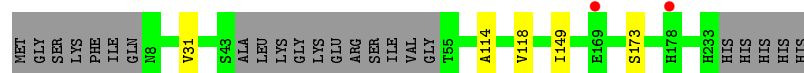
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	30	Total 30	O 30	0	0
4	C	21	Total 21	O 21	0	1
4	D	8	Total 8	O 8	0	0

- Molecule 1: Type II site-specific deoxyribonuclease



- Chain B:  88% 10%



- Chain C:  5% 94%



- Chain D: 4% 91% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.23Å 102.73Å 121.20Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	51.37 – 2.32 51.37 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.4 (51.37-2.32) 96.4 (51.37-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.216 , 0.258 0.214 , 0.257	Depositor DCC
R_{free} test set	1958 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.276 for -h,-k,l	Xtriage
Reported twinning fraction	0.694 for H, K, L 0.306 for -h,-k,l	Depositor
Outliers	0 of 37279 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7364	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: UNX, CA

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	0.41	0/1919	0.60	0/2592
1	B	0.39	0/1767	0.60	0/2389
1	C	0.38	0/1923	0.59	0/2596
1	D	0.39	0/1821	0.58	0/2461
All	All	0.40	0/7430	0.59	0/10038

There are no bond length outliers.

There are no bond angle outliers.

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	1874	0	1851	3	0
1	B	1727	0	1696	3	0
1	C	1879	0	1861	8	0
1	D	1781	0	1762	4	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
4	A	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	0	0	0
4	C	21	0	0	0	0
4	D	8	0	0	0	0
All	All	7364	0	7170	15	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 1.

All (15) 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:83:ASP:HB3	1:D:86:VAL:HG23	1.87	0.56
1:B:31:VAL:HG22	1:B:149:ILE:HD11	1.89	0.54
1:C:184[B]:LYS:HD2	1:C:184[B]:LYS:C	2.28	0.54
1:B:114:ALA:O	1:B:118:VAL:HG23	2.13	0.49
1:C:114:ALA:O	1:C:118:VAL:HG23	2.13	0.48
1:C:184[B]:LYS:HB3	1:C:184[B]:LYS:NZ	2.29	0.47
1:B:173:SER:HB2	1:C:11:GLU:HG3	1.98	0.46
1:A:135:TRP:CD2	1:A:150:TYR:HB2	2.50	0.46
1:C:115:GLU:OE2	1:D:108:HIS:NE2	2.43	0.46
1:A:13:ALA:HB2	1:A:32:ILE:HG13	2.00	0.43
1:C:130:ILE:HD11	1:C:148:PHE:CD1	2.55	0.42
1:A:114:ALA:O	1:A:118:VAL:HG23	2.20	0.42
1:C:93:TYR:HB2	1:D:222:LEU:HD22	2.02	0.41
1:C:166:ASP:HB3	1:C:186:PHE:CE1	2.56	0.41
1:D:130:ILE:HD11	1:D:148:PHE:CD1	2.56	0.40

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	231/238 (97%)	227 (98%)	4 (2%)	0	100	100
1	B	211/238 (89%)	206 (98%)	5 (2%)	0	100	100
1	C	232/238 (98%)	226 (97%)	6 (3%)	0	100	100
1	D	219/238 (92%)	213 (97%)	6 (3%)	0	100	100
All	All	893/952 (94%)	872 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	204/208 (98%)	203 (100%)	1 (0%)	88	95
1	B	189/208 (91%)	189 (100%)	0	100	100
1	C	205/208 (99%)	205 (100%)	0	100	100
1	D	195/208 (94%)	195 (100%)	0	100	100
All	All	793/832 (95%)	792 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is unknown and 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	233/238 (97%)	0.03	7 (3%) 50 57	43, 60, 93, 112	0
1	B	215/238 (90%)	0.02	2 (0%) 84 88	43, 65, 90, 108	0
1	C	233/238 (97%)	0.27	12 (5%) 27 34	55, 74, 101, 134	0
1	D	223/238 (93%)	0.32	9 (4%) 38 45	55, 82, 113, 129	0
All	All	904/952 (94%)	0.16	30 (3%) 46 53	43, 70, 104, 134	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	HIS	4.1
1	D	176	ILE	4.1
1	C	228	ILE	3.9
1	D	230	ALA	3.8
1	C	153	SER	3.2
1	A	226	ARG	3.2
1	D	75	PRO	3.1
1	A	206	LYS	3.0
1	C	202	SER	2.9
1	C	226	ARG	2.9
1	C	233	HIS	2.7
1	A	231	LEU	2.7
1	D	95	GLU	2.6
1	D	193	ARG	2.5
1	A	205	GLY	2.5
1	B	178	HIS	2.4
1	A	5	PHE	2.4
1	C	231	LEU	2.3
1	B	169	GLU	2.3
1	C	20	VAL	2.3
1	A	169	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	182	ILE	2.2
1	D	160	LEU	2.1
1	C	224	ALA	2.1
1	C	156	VAL	2.1
1	D	89	ILE	2.0
1	A	204	GLU	2.0
1	C	107	TRP	2.0
1	D	207	GLU	2.0
1	C	90	LEU	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
3	UNX	A	303	1/1	0.79	1.01	99,99,99,99	0
2	CA	D	302	1/1	0.81	0.06	107,107,107,107	0
2	CA	C	301	1/1	0.90	0.08	80,80,80,80	0
2	CA	A	302	1/1	0.97	0.09	85,85,85,85	0
2	CA	D	301	1/1	0.97	0.13	84,84,84,84	0
2	CA	A	301	1/1	0.97	0.09	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.