

# Full wwPDB X-ray Structure Validation Report (i)

#### Jul 25, 2023 – 12:43 AM EDT

PDB ID : 1BSU

Title : STRUCTURAL AND ENERGETIC ORIGINS OF INDIRECT READOUT

IN SITE-SPECIFIC DNA CLEAVAGE BY A RESTRICTION ENDONU-

CLEASE

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Deposited on : 1998-08-30

Resolution : 2.00 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) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

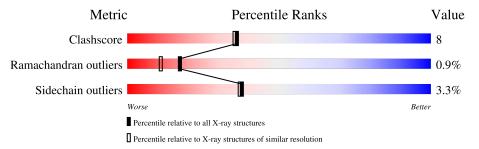
Validation Pipeline (wwPDB-VP) : 2.34

## 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 2.00 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain						
1	С	10	80%		20%	6			
2	D	11	36%	55%		9%			
3	A	244	75%		20%				
3	В	244	77%		16%	• 6%			



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4281 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 DNA chain called DNA (5'-D(P\*AP\*AP\*GP\*AP\*(5CM)P\*IP\*TP\*CP\*TP \*T)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	С	10	Total 205	C 99	N 36	O 60	P 10	0	0	0

• Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*AP\*AP\*GP\*AP\*(5CM)P\*IP\*TP\*CP\* TP\*T)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D	11	Total 222	C 109	N 41	O 62	P 10	0	0	0

• Molecule 3 is a protein called ENDONUCLEASE ECORV (3.1.21.4).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	A	236	10001	C 1197	- 1	O 349	S 1	0	0	0
3	В	229		C 1159	N 295	O 330	S 1	0	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	В	1	Total Ca 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	12	Total O 12 12	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	13	Total O 13 13	0	0
5	A	101	Total O 101 101	0	0
5	В	92	Total O 92 92	0	0



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

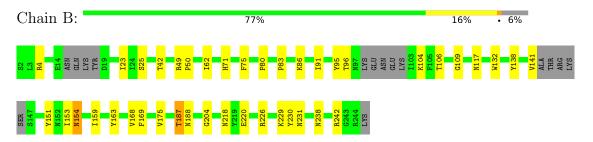
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.



• Molecule 1: DNA (5'-D(P\*AP\*AP\*GP\*AP\*(5CM)P\*IP\*TP\*CP\*TP\*T)-3') Chain C: 80% 20% • Molecule 2: DNA (5'-D(\*AP\*AP\*AP\*GP\*AP\*(5CM)P\*IP\*TP\*CP\*TP\*T)-3') Chain D: 36% • Molecule 3: ENDONUCLEASE ECORV (3.1.21.4) Chain A: 75% 20%

• Molecule 3: ENDONUCLEASE ECORV (3.1.21.4)





# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	50.30Å 64.00Å 49.10Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$109.10^{\circ}$ $108.10^{\circ}$ $96.50^{\circ}$	Depositor	
Resolution (Å)	6.00 - 2.00	Depositor	
% Data completeness	(Not available) (6.00-2.00)	Depositor	
(in resolution range)	(1100 available) (0.00 2.00)	-	
$R_{merge}$	0.09	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
$R, R_{free}$	0.183 , 0.258	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4281	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP	



## 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: 5CM, 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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	С	0.61	0/182	0.90	0/276	
2	D	0.62	0/202	0.92	0/308	
3	A	0.57	0/1899	0.76	2/2594~(0.1%)	
3	В	0.57	0/1831	0.76	$1/2496 \ (0.0\%)$	
All	All	0.57	0/4114	0.77	3/5674 (0.1%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	40	LEU	CA-CB-CG	-6.52	100.30	115.30
3	A	106	THR	N-CA-C	-5.73	95.52	111.00
3	В	106	THR	N-CA-C	-5.59	95.91	111.00

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	С	205	0	115	1	0
2	D	222	0	124	4	0
3	A	1849	0	1690	35	0
3	В	1785	0	1652	27	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	В	1	0	0	0	0
5	A	101	0	0	1	0
5	В	92	0	0	1	0
5	С	12	0	0	0	0
5	D	13	0	0	0	0
All	All	4281	0	3581	59	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 8.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
3:A:112:SER:HA	3:A:119:LYS:HE3	1.61	0.82
3:A:4:ARG:O	3:A:8:ILE:HG13	1.96	0.65
3:A:45:GLU:O	3:A:49:ARG:HG3	1.97	0.64
3:B:226:ARG:HB3	3:B:231:ASN:ND2	2.12	0.64
3:A:153:ILE:HD13	3:B:153:ILE:CG2	2.27	0.63
3:B:238:ASN:O	3:B:242:ARG:HG3	1.98	0.63
3:B:220:GLU:HB2	3:B:226:ARG:HG2	1.80	0.63
2:D:801:DA:H2"	2:D:802:DA:C8	2.34	0.63
3:A:153:ILE:HG21	3:B:153:ILE:HG21	1.84	0.59
3:A:62:ILE:HD12	3:A:78:TYR:CE2	2.39	0.58
3:A:153:ILE:HD13	3:B:153:ILE:HG21	1.88	0.55
3:A:49:ARG:HB2	3:A:50:PRO:HD3	1.89	0.55
3:A:116:ASN:O	3:A:118:THR:N	2.44	0.51
3:A:85:LYS:HA	3:A:129:ILE:HG23	1.93	0.49
3:A:121:ILE:HG12	3:A:123:TYR:O	2.11	0.49
3:B:168:VAL:HG22	3:B:169:PHE:N	2.28	0.49
3:A:31:TYR:HD2	3:B:50:PRO:HG2	1.78	0.48
3:A:114:ILE:HD12	3:A:217:ARG:HG3	1.94	0.48
2:D:803:DA:C6	2:D:804:DG:C6	3.02	0.47
2:D:810:DT:H5'	3:A:70:ASN:OD1	2.14	0.47
3:A:49:ARG:HG2	3:A:75:PHE:HZ	1.79	0.47
3:B:104:LYS:HD2	5:B:319:HOH:O	2.14	0.47
3:A:72:TYR:O	3:A:122:VAL:HG23	2.16	0.46
3:A:79:LYS:HE3	3:A:82:GLU:OE2	2.15	0.46
3:B:91:ILE:HD12	3:B:91:ILE:N	2.29	0.46
3:B:153:ILE:O	3:B:154:ASN:CB	2.63	0.46
3:A:119:LYS:NZ	5:A:383:HOH:O	2.49	0.46



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A		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	overlap (Å)
3:A:138:TYR:HA	3:A:165:GLY:O	2.15	0.46
2:D:805:DA:H2"	2:D:806:5CM:H5"	1.97	0.46
3:A:33:LEU:HB2	3:A:162:PRO:HG3	1.99	0.45
3:A:23:ILE:HG22	3:B:23:ILE:HG22	1.98	0.45
3:A:73:PRO:HG3	3:A:88:ALA:HB1	1.99	0.44
3:A:85:LYS:HA	3:A:129:ILE:CG2	2.48	0.44
3:A:133:ILE:HG13	3:A:176:ILE:HD11	1.99	0.44
3:A:20:VAL:HA	3:B:25:SER:HA	1.99	0.43
3:B:175:VAL:O	3:B:204:GLY:HA3	2.18	0.43
3:A:7:LEU:HD23	3:A:170:LEU:CD1	2.48	0.43
3:B:229:LYS:HB3	3:B:230:TYR:H	1.66	0.43
3:B:62:ILE:HD13	3:B:80:PRO:HD3	2.00	0.43
3:A:2:SER:N	3:A:5:SER:OG	2.51	0.43
3:B:151:TYR:CG	3:B:159:ILE:HG12	2.54	0.43
1:C:907:DI:O6	3:A:186:THR:HG21	2.19	0.42
3:A:95:TYR:HB3	3:A:138:TYR:CZ	2.55	0.42
3:A:170:LEU:C	3:A:170:LEU:HD23	2.40	0.42
3:B:83:PRO:O	3:B:86:LYS:HG3	2.20	0.42
3:B:95:TYR:HB3	3:B:138:TYR:CZ	2.55	0.42
3:A:55:ILE:O	3:A:59:HIS:HD2	2.03	0.42
3:B:109:GLY:HA2	3:B:187:THR:O	2.19	0.42
3:A:117:ASN:O	3:A:124:PRO:HA	2.20	0.42
3:B:163:TYR:CD1	3:B:163:TYR:O	2.73	0.41
3:B:49:ARG:HG2	3:B:75:PHE:CZ	2.56	0.41
3:A:49:ARG:HG2	3:A:75:PHE:CZ	2.55	0.41
3:B:226:ARG:HB3	3:B:231:ASN:HD21	1.86	0.41
3:B:151:TYR:CD2	3:B:159:ILE:HG12	2.56	0.41
3:A:40:LEU:HD23	3:A:40:LEU:HA	1.78	0.40
3:B:4:ARG:HB2	3:B:132:TRP:CH2	2.56	0.40
3:B:62:ILE:HD12	3:B:62:ILE:N	2.36	0.40
3:A:172:ASP:HB2	3:A:175:VAL:HG23	2.04	0.40
3:B:218:ASN:HB2	3:B:230:TYR:OH	2.22	0.40

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
3	A	232/244~(95%)	220 (95%)	11 (5%)	1 (0%)	34 30
3	В	221/244 (91%)	207 (94%)	11 (5%)	3 (1%)	11 5
All	All	453/488 (93%)	427 (94%)	22 (5%)	4 (1%)	17 11

#### All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	117	ASN
3	В	154	ASN
3	В	117	ASN
3	В	187	THR

#### 5.3.2 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		
3	A	184/220 (84%)	177 (96%)	7 (4%)	33 31		
3	В	177/220~(80%)	172 (97%)	5 (3%)	43 44		
All	All	361/440 (82%)	349 (97%)	12 (3%)	38 37		

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	70	ASN
3	A	71	HIS
3	A	118	THR
3	A	157	ASN
3	A	188	ASN
3	A	210	ASP
3	A	228	ASP
3	В	42	THR



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Mol	Chain	Res	Type
3	В	71	HIS
3	В	96	THR
3	В	141	VAL
3	В	188	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	69	GLN
3	В	71	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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		
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5CM	С	906	1	17,21,22	0.45	0	24,30,33	1.32	3 (12%)
2	5CM	D	806	2	17,21,22	0.47	0	24,30,33	1.25	2 (8%)

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	5CM	С	906	1	ı	0/7/21/22	0/2/2/2
2	5CM	D	806	2	-	2/7/21/22	0/2/2/2



There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	D	806	5CM	C2'-C1'-N1	-4.31	103.84	113.77
1	С	906	5CM	C2'-C1'-N1	-4.12	104.28	113.77
1	С	906	5CM	C5-C6-N1	-2.58	120.68	123.34
1	С	906	5CM	O3'-C3'-C4'	2.50	119.67	110.10
2	D	806	5CM	C5-C6-N1	-2.06	121.22	123.34

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	806	5CM	C3'-C4'-C5'-O5'
2	D	806	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	806	5CM	1	0

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (i)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

