



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XHV
Title : HincII bound to cleaved cognate DNA GTCGAC and Mn²⁺
Authors : Etzkorn, C.; Horton, N.C.
Deposited on : 2004-09-20
Resolution : 2.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

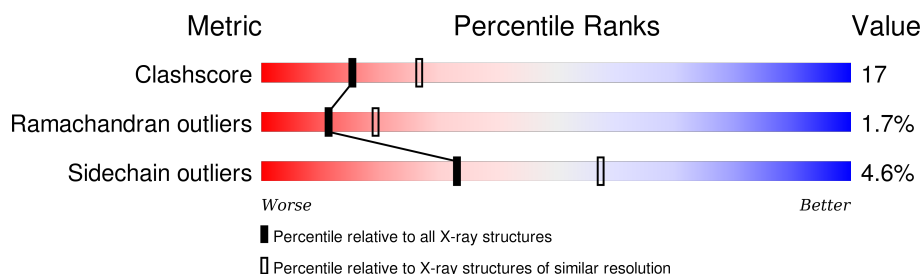
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	7	<div> <div>57%</div> <div>29%</div> <div>14%</div> </div>
1	G	7	<div> <div>29%</div> <div>43%</div> <div>29%</div> </div>
1	I	7	<div> <div>57%</div> <div>29%</div> <div>14%</div> </div>
1	K	7	<div> <div>14%</div> <div>57%</div> <div>14%</div> <div>14%</div> </div>
2	F	6	<div> <div>67%</div> <div>17%</div> <div>17%</div> </div>
2	H	6	<div> <div>50%</div> <div>33%</div> <div>17%</div> </div>
2	J	6	<div> <div>50%</div> <div>17%</div> <div>17%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	6	<div><div></div><div>100%</div></div>
3	A	257	<div><div></div><div>69%</div><div>27%</div><div></div><div></div></div>
3	B	257	<div><div></div><div>66%</div><div>30%</div><div></div><div></div></div>
3	C	257	<div><div></div><div>61%</div><div>32%</div><div></div><div></div></div>
3	D	257	<div><div></div><div>61%</div><div>31%</div><div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10198 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 5'-D(*GP*CP*CP*GP*GP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	7	Total	C	N	O	P	0	0	0
			140	67	26	41	6			
1	G	7	Total	C	N	O	P	0	0	0
			140	67	26	41	6			
1	I	7	Total	C	N	O	P	0	0	0
			140	67	26	41	6			
1	K	7	Total	C	N	O	P	0	0	0
			140	67	26	41	6			

- Molecule 2 is a DNA chain called 5'-D(P*GP*AP*CP*CP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	6	Total	C	N	O	P	0	0	0
			126	58	26	36	6			
2	H	6	Total	C	N	O	P	0	0	0
			126	58	26	36	6			
2	J	6	Total	C	N	O	P	0	0	0
			126	58	26	36	6			
2	L	6	Total	C	N	O	P	0	0	0
			126	58	26	36	6			

- Molecule 3 is a protein called Type II restriction enzyme HincII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	254	Total	C	N	O	S	0	0	0
			2058	1338	334	380	6			
3	B	252	Total	C	N	O	S	0	0	0
			2032	1322	330	374	6			
3	C	247	Total	C	N	O	S	0	0	0
			2005	1307	323	369	6			
3	D	247	Total	C	N	O	S	0	0	0
			1990	1296	319	369	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	THR	ARG	CONFLICT	UNP P17743
A	173	TRP	SER	CONFLICT	UNP P17743
B	130	THR	ARG	CONFLICT	UNP P17743
B	173	TRP	SER	CONFLICT	UNP P17743
C	130	THR	ARG	CONFLICT	UNP P17743
C	173	TRP	SER	CONFLICT	UNP P17743
D	130	THR	ARG	CONFLICT	UNP P17743
D	173	TRP	SER	CONFLICT	UNP P17743

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mn 1 1	0	0
4	J	3	Total Mn 3 3	0	0
4	D	3	Total Mn 3 3	0	0
4	H	3	Total Mn 3 3	0	0
4	B	3	Total Mn 3 3	0	0
4	C	3	Total Mn 3 3	0	0
4	A	2	Total Mn 2 2	0	0
4	L	2	Total Mn 2 2	0	0
4	F	2	Total Mn 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	217	Total O 217 217	0	0
5	B	302	Total O 302 302	0	0
5	C	160	Total O 160 160	0	0
5	D	198	Total O 198 198	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	21	Total 21	O 21	0	0
5	F	22	Total 22	O 22	0	0
5	G	29	Total 29	O 29	0	0
5	H	15	Total 15	O 15	0	0
5	I	18	Total 18	O 18	0	0
5	J	14	Total 14	O 14	0	0
5	K	16	Total 16	O 16	0	0
5	L	15	Total 15	O 15	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*C)-3'

Chain E: 



- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*C)-3'

Chain G: 

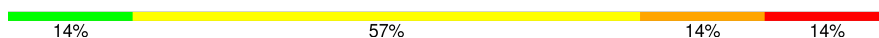


- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*C)-3'

Chain I: 



- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*C)-3'

Chain K: 



- Molecule 2: 5'-D(P*GP*AP*CP*CP*GP*G)-3'

Chain F: 



- Molecule 2: 5'-D(P*GP*AP*CP*CP*GP*G)-3'

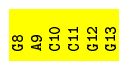
Chain H: 



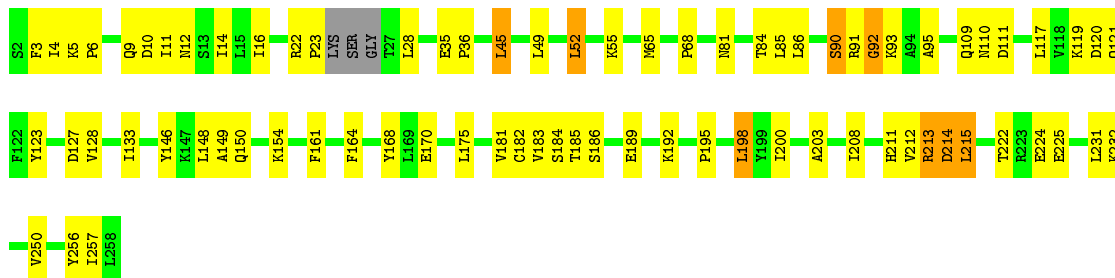
- Molecule 2: 5'-D(P*GP*AP*CP*CP*GP*G)-3'



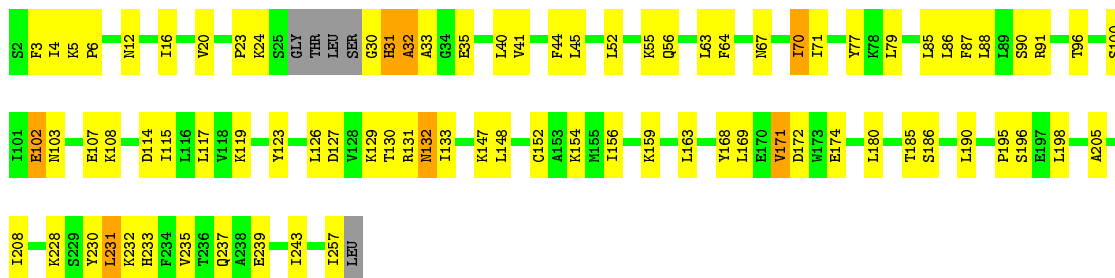
- Molecule 2: 5'-D(P*GP*AP*CP*CP*GP*G)-3'



- Molecule 3: Type II restriction enzyme HincII

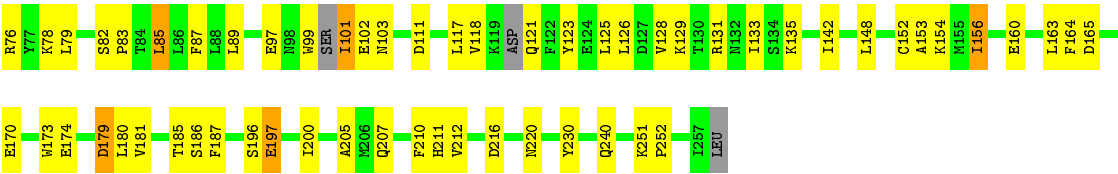


- Molecule 3: Type II restriction enzyme HincII

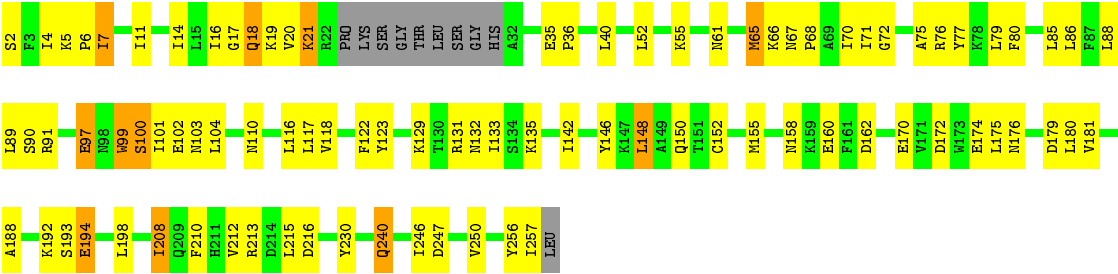


- Molecule 3: Type II restriction enzyme HincII





● Molecule 3: Type II restriction enzyme HincII



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.80 Å 178.20 Å 257.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	89.3 (50.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10198	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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: MN

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	E	0.67	0/156	0.85	1/239 (0.4%)
1	G	0.82	0/156	1.00	0/239
1	I	0.61	0/156	0.88	0/239
1	K	0.77	0/156	1.31	3/239 (1.3%)
2	F	1.05	1/141 (0.7%)	0.96	1/214 (0.5%)
2	H	0.97	1/141 (0.7%)	0.92	0/214
2	J	0.96	1/141 (0.7%)	0.92	1/214 (0.5%)
2	L	1.04	1/141 (0.7%)	1.18	0/214
3	A	0.51	0/2104	0.71	1/2843 (0.0%)
3	B	0.51	0/2079	0.70	1/2811 (0.0%)
3	C	0.47	0/2049	0.65	0/2766
3	D	0.49	0/2035	0.70	2/2755 (0.1%)
All	All	0.55	4/9455 (0.0%)	0.74	10/12987 (0.1%)

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	G	0	2
1	I	0	1
1	K	0	3
2	F	0	2
2	H	0	2
2	J	0	2
2	L	0	1
3	B	0	1
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	8	DG	OP3-P	-7.11	1.52	1.61
2	H	8	DG	OP3-P	-7.03	1.52	1.61
2	J	8	DG	OP3-P	-6.64	1.53	1.61
2	F	8	DG	OP3-P	-6.60	1.53	1.61

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	55	LYS	N-CA-C	-6.10	94.52	111.00
1	E	7	DC	C2'-C3'-O3'	-6.07	92.58	112.60
3	A	213	ARG	N-CA-C	-6.00	94.81	111.00
3	D	65	MET	N-CA-C	-5.94	94.97	111.00
3	D	55	LYS	N-CA-C	-5.70	95.61	111.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	8	DG	Sidechain
2	F	9	DA	Sidechain
1	G	1	DG	Sidechain
1	G	2	DC	Sidechain
2	H	8	DG	Sidechain

5.2 Too-close contacts ⓘ

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	E	140	0	80	2	0
1	G	140	0	79	8	0
1	I	140	0	79	4	0
1	K	140	0	80	3	0
2	F	126	0	67	2	0
2	H	126	0	67	3	0
2	J	126	0	67	7	0
2	L	126	0	67	4	0
3	A	2058	0	2027	61	0
3	B	2032	0	1985	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2005	0	1966	78	0
3	D	1990	0	1928	79	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
4	J	3	0	0	0	0
4	L	2	0	0	0	0
5	A	217	0	0	11	4
5	B	302	0	0	10	3
5	C	160	0	0	11	2
5	D	198	0	0	10	0
5	E	21	0	0	1	0
5	F	22	0	0	4	0
5	G	29	0	0	1	0
5	H	15	0	0	1	0
5	I	18	0	0	1	0
5	J	14	0	0	0	0
5	K	16	0	0	0	0
5	L	15	0	0	0	0
All	All	10198	0	8492	305	9

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 17.

The worst 5 of 305 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)
2:J:8:DG:H2''	2:J:9:DA:H5''	1.40	1.01
3:B:56:GLN:HG2	5:B:1164:HOH:O	1.67	0.93
3:A:92:GLY:N	5:A:1127:HOH:O	2.00	0.92
3:C:19:LYS:HG2	3:C:181:VAL:HG22	1.52	0.89
3:D:175:LEU:H	3:D:175:LEU:HD23	1.39	0.86

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1118:HOH:O	5:A:1118:HOH:O[6_555]	1.33	0.87
5:A:1189:HOH:O	5:A:1189:HOH:O[8_556]	1.50	0.70
5:B:1229:HOH:O	5:B:1229:HOH:O[7_557]	1.64	0.56
5:C:1128:HOH:O	5:C:1128:HOH:O[7_657]	1.82	0.38
5:B:1273:HOH:O	5:B:1273:HOH:O[8_556]	1.93	0.27

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	250/257 (97%)	232 (93%)	14 (6%)	4 (2%)	12	21
3	B	248/257 (96%)	228 (92%)	15 (6%)	5 (2%)	9	15
3	C	239/257 (93%)	216 (90%)	20 (8%)	3 (1%)	15	26
3	D	243/257 (95%)	219 (90%)	19 (8%)	5 (2%)	9	14
All	All	980/1028 (95%)	895 (91%)	68 (7%)	17 (2%)	11	19

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	32	ALA
3	C	197	GLU
3	D	21	LYS
3	D	100	SER
3	A	214	ASP

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	219/229 (96%)	210 (96%)	9 (4%)	37	63
3	B	214/229 (93%)	206 (96%)	8 (4%)	41	68
3	C	213/229 (93%)	203 (95%)	10 (5%)	32	56
3	D	208/229 (91%)	196 (94%)	12 (6%)	25	45
All	All	854/916 (93%)	815 (95%)	39 (5%)	33	57

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	LYS
3	C	101	ILE
3	D	208	ILE
3	C	52	LEU
3	C	63	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	132	ASN
3	B	176	ASN
3	D	109	GLN
3	B	103	ASN
3	D	110	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 22 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.