

wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 11:22 AM EST

PDB ID : 1AZ0

Title : ECORV ENDONUCLEASE/DNA COMPLEX

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Deposited on : 1997-11-24

Resolution : 2.00 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
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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

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)

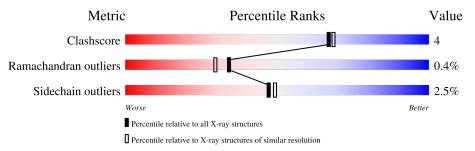
Validation Pipeline (wwPDB-VP) : 2.36

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	11	55%	36% 9%	_			
1	D	11	55%	36% 9%	_			
2	A	244	78%	17% •	-			
2	В	244	73%	19% • 6%	/ 6			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4296 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(*AP*AP*AP*AP*TP*AP*TP*CP*TP* T)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	C	11	Total	С	N	О	Р	0	0	0
1		11	223	109	41	63	10	0	U	U
1	D	11	Total	С	N	О	Р	0	0	0
1	ש	11	223	109	41	63	10		U	U

• Molecule 2 is a protein called PROTEIN (TYPE II RESTRICTION ENZYME ECORV).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	Λ	237	Total	С	N	О	S	0	0	0
	A	231	1838	1192	301	344	1	0	U	0
9	D	229	Total	С	N	О	S	0	0	0
2	D	229	1781	1158	295	327	1	0	U	U

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	В	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	15	Total O 15 15	0	0
4	D	13	Total O 13 13	0	0
4	A	108	Total O 108 108	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	93	Total O 93 93	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. 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.



Chain C: 55% 36% 9%

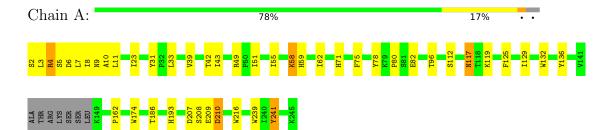
A902 A902 A905 T906 A907

• Molecule 1: DNA (5'-D(*AP*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3')

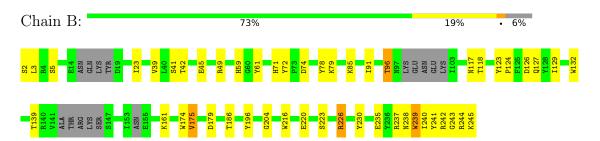
Chain D: 55% 36% 9%

A802 A802 A805 T806 A807

• Molecule 2: PROTEIN (TYPE II RESTRICTION ENZYME ECORV)



• Molecule 2: PROTEIN (TYPE II RESTRICTION ENZYME ECORV)





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	49.00Å 50.20Å 64.10Å	Depositor	
a, b, c, α , β , γ	109.00° 108.00° 96.00°	Depositor	
Resolution (Å)	6.00 - 2.00	Depositor	
% Data completeness	88.0 (6.00-2.00)	Depositor	
(in resolution range)	00.0 (0.00 2.00)	Depositor	
R_{merge}	0.07	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.184 , 0.246	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4296	wwPDB-VP	
Average B, all atoms (Å ²)	27.0	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: 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	Chain	RMSZ $ \# Z > 5$		RMSZ	# Z > 5	
1	С	0.43	0/250	0.91	0/384	
1	D	0.45	0/250	0.96	0/384	
2	A	0.83	0/1888	1.41	$16/2580 \; (0.6\%)$	
2	В	0.82	0/1826	1.43	$21/2487 \; (0.8\%)$	
All	All	0.79	0/4214	1.36	37/5835~(0.6%)	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	В	239	TRP	CD1-CG-CD2	9.21	113.66	106.30
2	В	174	TRP	CD1-CG-CD2	8.61	113.19	106.30
2	A	132	TRP	CD1-CG-CD2	7.97	112.68	106.30
2	A	174	TRP	CD1-CG-CD2	7.63	112.41	106.30
2	В	239	TRP	CE2-CD2-CG	-7.60	101.22	107.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	С	906	DT	Sidechain
1	D	806	DT	Sidechain

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	223	0	127	7	0
1	D	223	0	127	4	0
2	A	1838	0	1669	12	142
2	В	1781	0	1652	13	172
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	A	108	0	0	0	39
4	В	93	0	0	1	9
4	С	15	0	0	0	0
4	D	13	0	0	0	0
All	All	4296	0	3575	29	181

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 4.

The worst 5 of 29 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:C:901:DA:H2'	1:C:902:DA:C8	2.06	0.90
2:A:112:SER:HA	2:A:119:LYS:HE2	1.60	0.83
2:A:62:ILE:HD11	2:A:80:PRO:HG3	1.65	0.79
1:C:901:DA:C2'	1:C:902:DA:C8	2.72	0.73
1:C:901:DA:H2"	1:C:902:DA:O4'	2.03	0.59

The worst 5 of 181 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)
2:B:85:LYS:CA	4:A:391:HOH:O[1_554]	0.27	1.93

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:A:7:LEU:N	2:B:242:ARG:CA[1_666]	0.39	1.81
2:A:9:ASN:N	2:B:243:GLY:CA[1_666]	0.48	1.72
2:A:9:ASN:ND2	2:B:244:ARG:CB[1_666]	0.53	1.67
2:A:5:SER:CB	2:B:245:LYS:C[1_666]	0.55	1.65

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	Perce	ntiles
2	A	233/244 (96%)	224 (96%)	8 (3%)	1 (0%)	34	30
2	В	219/244 (90%)	213 (97%)	5 (2%)	1 (0%)	29	23
All	All	452/488 (93%)	437 (97%)	13 (3%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	117	ASN
2	В	117	ASN

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.

\mathbf{M}	ol	Chain	Analysed	Rotameric	Outliers	Percentiles
2)	A	179/220 (81%)	173 (97%)	6 (3%)	37 36
2)	В	176/220 (80%)	173 (98%)	3 (2%)	60 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	355/440 (81%)	346 (98%)	9 (2%)	47 49

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	71	HIS
2	В	96	THR
2	A	96	THR
2	A	129	ILE
2	A	210	ASP

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

Mol	Chain	Res	Type
2	A	15	ASN

5.3.3 RNA (i)

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 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.

