



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:49 AM UTC

PDB ID : 1EO4 / pdb_00001eo4
Title : ECORV BOUND TO MN2+ AND COGNATE DNA CONTAINING A 3'S
SUBSTITUTION AT THE CLEAVAGE SITE
Authors : Horton, N.C.; Connolly, B.A.; Perona, J.J.
Deposited on : 2000-03-21
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

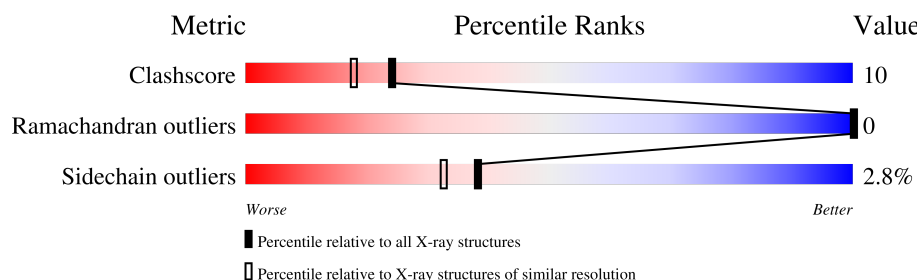
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	11	36% 45% 9% 9%
1	D	11	9% 27% 55% 9%
2	A	245	76% 19% • •
2	B	245	77% 18% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4512 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(*CP*AP*AP*GP*AP*(TSP)P*AP*TP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	10	Total	C	N	O	P	S	0	0	0
			205	99	36	59	10	1			
1	D	10	Total	C	N	O	P	S	0	0	0
			201	98	37	56	9	1			

- Molecule 2 is a protein called TYPE II RESTRICTION ENZYME ECORV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	238	Total	C	N	O	S		0	0	0
			1899	1227	314	357	1				
2	B	236	Total	C	N	O	S		0	0	0
			1894	1225	312	356	1				

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mn	0	0
			4	4		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	21	Total	O	0	0
			21	21		
5	D	29	Total	O	0	0
			29	29		
5	A	137	Total	O	0	0
			137	137		
5	B	113	Total	O	0	0
			113	113		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.70 Å 48.50 Å 63.70 Å 96.70° 109.60° 106.30°	Depositor
Resolution (Å)	4.90 – 1.90	Depositor
% Data completeness (in resolution range)	96.6 (4.90-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.213 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4512	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, MN, TSP

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	C	0.42	0/206	0.87	0/313
1	D	0.48	0/202	1.13	2/307 (0.7%)
2	A	0.77	0/1947	1.04	7/2643 (0.3%)
2	B	0.79	0/1943	1.04	12/2640 (0.5%)
All	All	0.75	0/4298	1.04	21/5903 (0.4%)

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	C	0	1
1	D	0	4
All	All	0	5

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	THR	N-CA-C	-7.44	97.45	109.96
2	A	221	ARG	N-CA-C	7.33	120.33	111.82
1	D	4	DG	C4'-C3'-O3'	-6.46	100.31	110.00
2	A	17	LYS	N-CA-C	6.32	120.99	113.28
2	B	233	ILE	N-CA-C	6.21	116.38	110.42
2	B	67	LYS	N-CA-C	-6.20	104.77	112.90
2	B	240	ILE	CB-CA-C	-6.05	104.22	111.97
2	B	3	LEU	N-CA-C	-6.05	104.68	111.28
2	B	221	ARG	N-CA-C	5.98	118.76	111.82
2	B	153	ILE	N-CA-C	5.63	117.04	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	DA	C4'-C3'-O3'	-5.55	101.68	110.00
2	A	106	THR	N-CA-C	-5.28	100.69	109.46
2	B	49	ARG	N-CA-C	5.21	121.31	109.81
2	B	97	ASN	N-CA-C	-5.17	107.14	112.93
2	B	119	LYS	N-CA-C	5.13	116.67	108.41
2	A	67	LYS	N-CA-C	-5.12	105.39	111.69
2	A	30	ILE	N-CA-C	5.10	115.31	108.17
2	A	161	LYS	CA-C-N	5.06	126.17	119.84
2	A	161	LYS	C-N-CA	5.06	126.17	119.84
2	B	79	LYS	CA-C-N	5.01	124.73	119.82
2	B	79	LYS	C-N-CA	5.01	124.73	119.82

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	10	DT	Sidechain
1	D	10	DT	Sidechain
1	D	5	DA	Sidechain
1	D	7	DA	Sidechain
1	D	8	DT	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	C	205	0	115	7	0
1	D	201	0	115	19	0
2	A	1899	0	1780	35	0
2	B	1894	0	1779	31	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	137	0	0	5	0
5	B	113	0	0	1	0
5	C	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	29	0	0	1	0
All	All	4512	0	3795	80	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 10.

All (80) 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:A:153:ILE:HD12	2:B:153:ILE:HD12	1.56	0.87
1:D:3:DA:H2''	1:D:4:DG:C5'	2.18	0.73
2:B:49:ARG:HG2	2:B:75:PHE:HZ	1.52	0.72
2:A:220:GLU:HB2	2:A:226:ARG:HG2	1.71	0.72
1:D:2:DA:H2''	1:D:3:DA:O5'	1.92	0.70
2:A:14:GLU:HG2	2:A:51:ILE:HD11	1.76	0.66
2:A:97:ASN:HB2	5:A:664:HOH:O	1.97	0.65
1:D:7:DA:H2''	1:D:8:DT:O5'	1.97	0.65
2:B:85:LYS:HB3	2:B:129:ILE:HD13	1.79	0.63
2:A:220:GLU:HB2	2:A:226:ARG:CG	2.29	0.62
2:B:8:ILE:HG12	2:B:170:LEU:HB3	1.80	0.62
2:B:49:ARG:HG2	2:B:75:PHE:CZ	2.33	0.62
1:D:2:DA:H2''	1:D:3:DA:C5'	2.30	0.61
2:A:69:GLN:HB3	5:A:738:HOH:O	1.99	0.61
2:A:72:TYR:O	2:A:121:ILE:HA	2.00	0.61
2:B:102:LYS:HB3	2:B:193:HIS:NE2	2.16	0.60
2:B:23:ILE:CG1	2:B:31:TYR:HB2	2.31	0.60
2:A:141:VAL:HG21	2:A:164:LYS:HG3	1.83	0.60
1:D:1:DC:H5''	2:A:180:LEU:HD13	1.84	0.60
1:C:2:DA:H3'	2:B:223:SER:OG	2.02	0.59
2:A:146:SER:HB2	2:A:160:PRO:HG3	1.85	0.59
2:B:91:ILE:HD13	2:B:134:ILE:HB	1.84	0.59
2:B:53:ASN:O	2:B:57:GLU:HG3	2.02	0.59
2:A:80:PRO:HD2	5:A:728:HOH:O	2.02	0.59
1:D:7:DA:C2'	1:D:8:DT:O5'	2.51	0.59
2:A:141:VAL:CG2	2:A:164:LYS:HG3	2.33	0.59
2:B:121:ILE:HG12	2:B:123:TYR:O	2.03	0.58
2:B:29:LYS:HE2	2:B:150:THR:HG21	1.84	0.58
1:D:3:DA:H2''	1:D:4:DG:O4'	2.03	0.58
1:D:4:DG:H2''	1:D:5:DA:O5'	2.03	0.57
1:D:1:DC:H2''	1:D:2:DA:C8	2.39	0.57
2:A:146:SER:CB	2:A:160:PRO:HG3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:12:TYR:O	2:A:16:GLN:HG2	2.06	0.55
2:A:45:GLU:HG3	2:A:91:ILE:HD12	1.88	0.55
2:A:45:GLU:O	2:A:49:ARG:HG3	2.07	0.54
2:B:8:ILE:HG23	5:B:708:HOH:O	2.08	0.53
2:A:195:HIS:HD2	5:A:638:HOH:O	1.90	0.53
1:D:5:DA:OP1	2:B:119:LYS:NZ	2.37	0.53
1:D:3:DA:H2''	1:D:4:DG:H5'	1.90	0.53
1:D:9:DC:H1'	2:A:70:ASN:ND2	2.23	0.53
1:D:3:DA:H2''	1:D:4:DG:O5'	2.09	0.53
2:B:96:THR:O	2:B:139:THR:HA	2.08	0.53
2:A:23:ILE:CD1	2:B:23:ILE:HG22	2.39	0.52
1:C:7:DA:H2''	1:C:8:DT:C5'	2.39	0.51
2:B:23:ILE:HG13	2:B:31:TYR:HB2	1.91	0.51
2:B:31:TYR:N	2:B:31:TYR:CD1	2.79	0.51
1:C:5:DA:H2''	1:C:6:TSP:H5'	1.93	0.51
1:D:8:DT:H2'	1:D:9:DC:C6	2.46	0.51
2:A:61:TYR:CZ	2:A:79:LYS:HD2	2.46	0.51
2:A:29:LYS:HE2	2:A:150:THR:HG21	1.94	0.50
1:D:7:DA:H62	2:B:186:THR:HG21	1.77	0.50
2:A:23:ILE:HD13	2:B:23:ILE:HG22	1.92	0.50
1:D:1:DC:H5''	2:A:180:LEU:CD1	2.42	0.50
2:B:183:SER:OG	2:B:188:ASN:HB2	2.12	0.49
1:C:7:DA:H2''	1:C:8:DT:H5''	1.95	0.49
2:B:118:THR:HG22	2:B:118:THR:O	2.13	0.49
1:D:2:DA:C2'	1:D:3:DA:O5'	2.60	0.48
1:D:9:DC:H1'	2:A:70:ASN:HD21	1.78	0.48
1:C:6:TSP:H4'	2:A:70:ASN:C	2.39	0.48
2:B:51:ILE:N	2:B:51:ILE:HD13	2.28	0.48
1:D:10:DT:H1'	5:D:124:HOH:O	2.13	0.47
2:A:31:TYR:CD1	2:A:31:TYR:N	2.83	0.46
2:B:113:PHE:HA	2:B:116:ASN:O	2.15	0.46
2:B:39:VAL:O	2:B:43:ILE:HG12	2.16	0.46
2:B:169:PHE:C	2:B:169:PHE:CD1	2.95	0.45
2:B:153:ILE:O	2:B:156:LEU:HG	2.17	0.45
2:A:113:PHE:HA	2:A:116:ASN:O	2.17	0.45
2:A:19:ASP:OD2	2:A:161:LYS:HE3	2.17	0.44
2:B:78:TYR:HB3	2:B:86:LYS:HG2	2.00	0.44
2:B:102:LYS:HE3	2:B:193:HIS:CE1	2.52	0.44
1:C:6:TSP:H73	2:A:186:THR:HB	1.99	0.44
2:A:183:SER:OG	2:A:188:ASN:HB2	2.17	0.43
2:A:20:VAL:HG12	2:A:33:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:25:SER:HB2	2:A:27:GLU:OE1	2.21	0.41
2:A:158:GLU:HB2	5:A:723:HOH:O	2.20	0.41
2:B:102:LYS:HB3	2:B:193:HIS:CD2	2.56	0.41
1:C:5:DA:H2''	1:C:6:TSP:C5'	2.51	0.41
2:B:88:ALA:HB2	2:B:128:TYR:CD2	2.56	0.41
2:A:151:TYR:CG	2:A:159:ILE:HG12	2.57	0.40
2:A:159:ILE:HA	2:A:160:PRO:HD2	1.94	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	
2	A	230/245 (94%)	220 (96%)	10 (4%)	0	100	100
2	B	230/245 (94%)	222 (96%)	8 (4%)	0	100	100
All	All	460/490 (94%)	442 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	194/221 (88%)	187 (96%)	7 (4%)	31	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/221 (88%)	190 (98%)	4 (2%)	47	44
All	All	388/442 (88%)	377 (97%)	11 (3%)	38	32

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	31	TYR
2	A	40	LEU
2	A	114	ILE
2	A	129	ILE
2	A	170	LEU
2	A	188	ASN
2	A	221	ARG
2	B	40	LEU
2	B	51	ILE
2	B	137	VAL
2	B	188	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	9	ASN
2	A	53	ASN
2	A	157	ASN
2	A	188	ASN
2	A	195	HIS
2	B	195	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TSP	C	6	1	17,21,22	0.41	0	21,30,33	0.90	1 (4%)
1	TSP	D	6	1	17,21,22	0.53	0	21,30,33	0.57	0

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	TSP	C	6	1	-	3/7/21/22	0/2/2/2
1	TSP	D	6	1	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	TSP	C2'-C1'-N1	-2.78	106.85	113.81

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	6	TSP	C2'-C1'-N1-C6
1	C	6	TSP	O4'-C1'-N1-C6
1	C	6	TSP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	6	TSP	4	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	$\# Z > 2$
4	ACY	B	602	-	3,3,3	0.82	0	3,3,3	5.57	2 (66%)
4	ACY	A	601	-	3,3,3	1.17	0	3,3,3	5.95	2 (66%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	601	ACY	OXT-C-CH3	7.62	147.02	115.05
4	B	602	ACY	O-C-CH3	7.41	152.92	122.53
4	A	601	ACY	O-C-CH3	-6.88	94.32	122.53
4	B	602	ACY	OXT-C-O	-5.84	100.38	122.03

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.