



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:15 PM GMT

PDB ID : 1EO4
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
<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

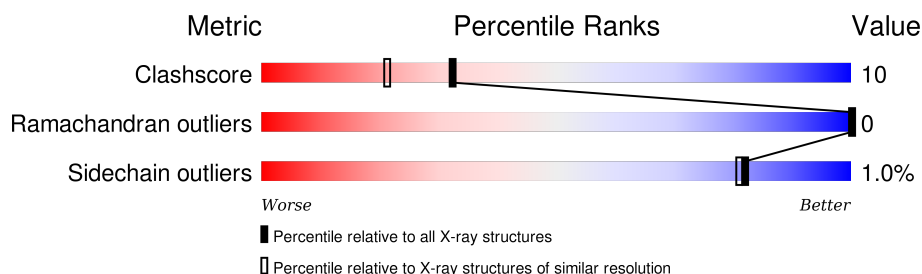
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 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	C	11	
1	D	11	
2	A	245	
2	B	245	

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 (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is ACETIC ACID (three-letter code: 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	A	137	Total	O	0	0
			137	137		
5	B	113	Total	O	0	0
			113	113		
5	C	21	Total	O	0	0
			21	21		
5	D	29	Total	O	0	0
			29	29		

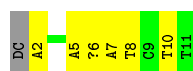
3 Residue-property plots [i](#)

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: DNA (5'-D(*CP*AP*AP*GP*AP*(TSP)P*AP*TP*CP*TP*T)-3')

Chain C: 




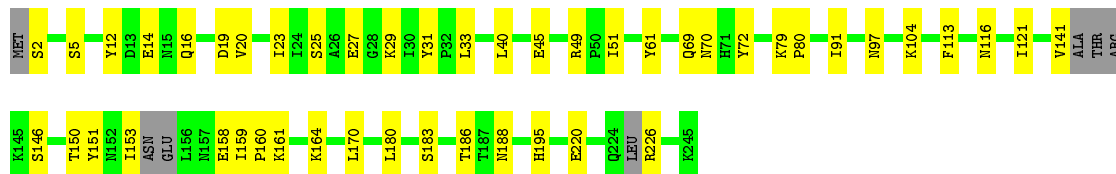
- Molecule 1: DNA (5'-D(*CP*AP*AP*GP*AP*(TSP)P*AP*TP*CP*TP*T)-3')

Chain D: 




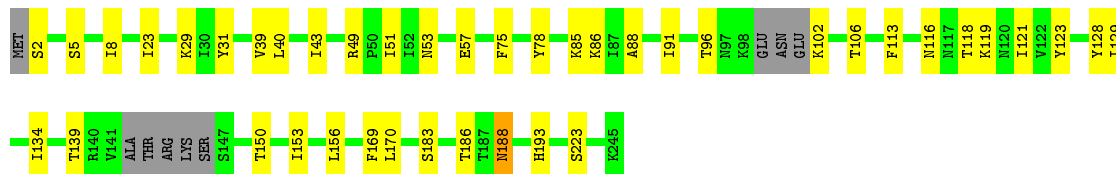
- Molecule 2: TYPE II RESTRICTION ENZYME ECVRV

Chain A: 



- Molecule 2: TYPE II RESTRICTION ENZYME ECVRV

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.65	0/206	0.83	0/313
1	D	0.92	0/202	1.19	2/307 (0.7%)
2	A	0.65	0/1947	0.75	0/2643
2	B	0.66	0/1943	0.78	1/2640 (0.0%)
All	All	0.67	0/4298	0.80	3/5903 (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	C	0	1
1	D	0	4
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	DT	O4'-C1'-C2'	5.37	110.19	105.90
1	D	4	DG	O4'-C1'-C2'	5.04	109.93	105.90
2	B	106	THR	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	10	DT	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	20	0
2	A	1899	0	1780	37	0
2	B	1894	0	1779	33	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	6	0
5	B	113	0	0	1	0
5	C	21	0	0	0	0
5	D	29	0	0	1	0
All	All	4512	0	3795	84	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 (84) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:ARG:HG2	2:B:75:PHE:CZ	2.33	0.62
2:B:8:ILE:HG12	2:B:170:LEU:HB3	1.80	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
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
1:C:2:DA:H3'	2:B:223:SER:OG	2.02	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
1:C:6:TSP:H73	2:A:186:THR:HB	1.88	0.56
2:B:2:SER:N	2:B:5:SER:HG	2.04	0.55
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:2:SER:N	2:A:5:SER:HG	2.08	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
2:A:104:LYS:NZ	5:A:684:HOH:O	2.45	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:O	2:B:118:THR:HG22	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
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:N	2:A:31:TYR:CD1	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: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:102:LYS:HE3	2:B:193:HIS:CE1	2.52	0.44
2:B:78:TYR:HB3	2:B:86:LYS:HG2	2.00	0.44
2:A:183:SER:OG	2:A:188:ASN:HB2	2.17	0.43
1:C:6:TSP:H4'	2:A:70:ASN:C	2.39	0.43
2:A:20:VAL:HG12	2:A:33:LEU:HD11	2.02	0.41
2:A:25:SER:HB2	2:A:27:GLU:OE1	2.21	0.41
1:D:6:TSP:H73	2:B:186:THR:HB	2.02	0.41
2:B:102:LYS:HB3	2:B:193:HIS:CD2	2.56	0.41
2:A:158:GLU:HB2	5:A:723:HOH:O	2.20	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
2:B:169:PHE:CD1	2:B:169:PHE:C	2.95	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	
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

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%)	192 (99%)	2 (1%)	82	81
2	B	194/221 (88%)	192 (99%)	2 (1%)	82	81
All	All	388/442 (88%)	384 (99%)	4 (1%)	82	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	40	LEU
2	A	170	LEU
2	B	40	LEU
2	B	188	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	9	ASN
2	A	157	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	10,21,22	1.42	3 (30%)	11,30,33	5.05	3 (27%)
1	TSP	D	6	1	10,21,22	1.23	3 (30%)	11,30,33	5.31	3 (27%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	TSP	C6-C5	-2.39	1.33	1.40
1	D	6	TSP	C6-C5	-2.14	1.34	1.40
1	C	6	TSP	C6-N1	2.04	1.38	1.35
1	D	6	TSP	C6-N1	2.05	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	6	TSP	C4-N3	2.34	1.37	1.33
1	C	6	TSP	C4-N3	2.93	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6	TSP	C5-C4-N3	-9.34	114.74	125.14
1	C	6	TSP	C5-C4-N3	-8.91	115.22	125.14
1	C	6	TSP	C2'-C1'-N1	-3.00	106.85	114.16
1	D	6	TSP	C5M-C5-C6	2.15	122.95	118.62
1	C	6	TSP	C4-N3-C2	13.58	126.98	115.25
1	D	6	TSP	C4-N3-C2	14.70	127.95	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	601	-	1,3,3	4.63	1 (100%)	0,3,3	0.00	-
4	ACY	B	602	-	1,3,3	1.67	0	0,3,3	0.00	-

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
4	ACY	A	601	-	-	0/0/0/0	0/0/0/0
4	ACY	B	602	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	ACY	CH3-C	4.63	1.55	1.48

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 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.