



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:03 PM UTC

PDB ID : 2V16 / pdb_00002v16
Title : Crystal Structure of Renin with Inhibitor 3
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Deposited on : 2007-05-22
Resolution : 2.80 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 ⓘ 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**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

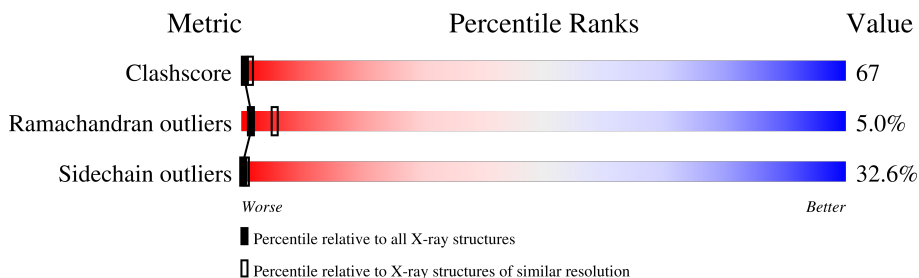
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

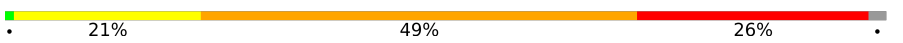
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	340	
1	O	340	

2 Entry composition [i](#)

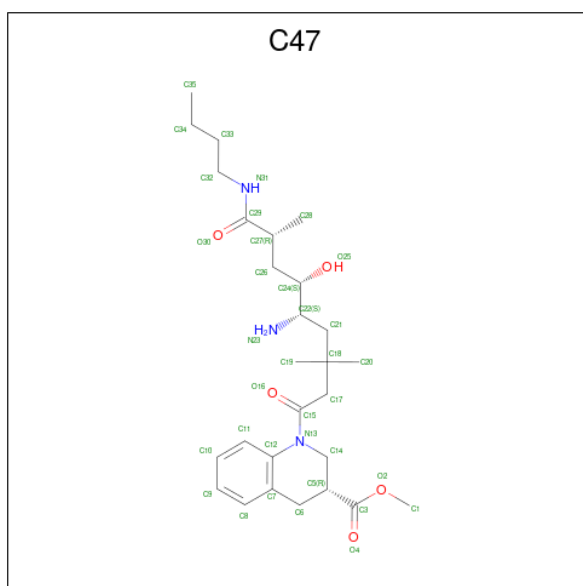
There are 3 unique types of molecules in this entry. The entry contains 5216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein called RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	334	Total	C	N	O	S	0	0	1
			2567	1639	416	498	14			
1	O	332	Total	C	N	O	S	0	0	1
			2557	1634	414	495	14			

- Molecule 2 is METHYL (3R)-1-[(5S,6S,8R)-5-AMINO-9-BUTYLAMINO-6-HYDROXY-3,3,8-TRIMETHYL-9-OXO-NONANOYL]-3,4-DIHYDRO-2H-QUINOLINE-3-CARBOXYLATE (CCD ID: C47) (formula: $C_{27}H_{43}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			35	27	3	5		
2	O	1	Total	C	N	O	0	0
			35	27	3	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	15	Total 15	O 15	0	0
3	O	7	Total 7	O 7	0	0

H287	A288	M289	D290	T291	P292	P293	P294	T295	G296	P297	T298	W299	A300	L301	G302	A303	T304	F305	I306	R307	R308	F309	Y310	T311	E312	F313	D314	R315	R316	N317	N318	R319	I320	G321	F322	A323	L324	A325	R326
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	142.90 Å 142.90 Å 142.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: C47

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	5.36	762/2626 (29.0%)	4.40	819/3560 (23.0%)
1	O	5.13	694/2616 (26.5%)	4.57	837/3547 (23.6%)
All	All	5.25	1456/5242 (27.8%)	4.48	1656/7107 (23.3%)

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	2	2
1	O	5	3
All	All	7	5

The worst 5 of 1456 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	316	ARG	CZ-NH1	28.15	1.72	1.32
1	C	293	PRO	C-O	27.16	1.54	1.24
1	C	287	HIS	ND1-CE1	26.99	1.59	1.32
1	C	157	ARG	NE-CZ	26.06	1.61	1.33
1	C	240	ARG	CZ-NH2	25.54	1.66	1.33

The worst 5 of 1656 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	74	ARG	NE-CZ-NH2	24.68	141.41	119.20
1	C	244	ASP	CA-CB-CG	23.85	136.45	112.60
1	C	320	ILE	CA-C-N	-23.09	100.03	122.66
1	C	320	ILE	C-N-CA	-23.09	100.03	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	178	ASN	CA-CB-CG	-21.85	90.75	112.60

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	182	ILE	CB
1	C	311	THR	CB
1	O	156	ASN	CA
1	O	183	ASN	CA
1	O	202	SER	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	154	TYR	Sidechain
1	C	220	TYR	Sidechain
1	O	157	ARG	Mainchain
1	O	272	ALA	Mainchain
1	O	310	TYR	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	2567	0	2499	310	0
1	O	2557	0	2493	373	0
2	C	35	0	43	11	0
2	O	35	0	43	15	0
3	C	15	0	0	3	0
3	O	7	0	0	2	0
All	All	5216	0	5078	685	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 67.

The worst 5 of 685 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)
1:C:186:LYS:CE	1:C:186:LYS:CD	1.75	1.64
1:C:186:LYS:CD	1:C:186:LYS:CG	1.76	1.61
1:O:204:LEU:CB	1:O:204:LEU:CG	1.79	1.60
1:C:281(C):LYS:CD	1:C:281(C):LYS:CE	1.76	1.59
1:O:173:GLN:CG	1:O:173:GLN:CB	1.76	1.59

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	
1	C	330/340 (97%)	283 (86%)	34 (10%)	13 (4%)	2	8
1	O	328/340 (96%)	274 (84%)	34 (10%)	20 (6%)	1	3
All	All	658/680 (97%)	557 (85%)	68 (10%)	33 (5%)	1	5

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	185	ILE
1	C	207	GLU
1	C	234	ALA
1	C	235	LEU
1	C	240	ARG

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	
1	C	283/290 (98%)	200 (71%)	83 (29%)	0	1
1	O	282/290 (97%)	181 (64%)	101 (36%)	0	0
All	All	565/580 (97%)	381 (67%)	184 (33%)	0	1

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	90	THR
1	O	202	SER
1	O	118	ASP
1	O	152	SER
1	O	227	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	191	GLN
1	O	318	ASN
1	O	287	HIS
1	C	318	ASN
1	O	178	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	$\# Z > 2$
2	C47	O	1327	-	35,36,36	4.08	20 (57%)	39,50,50	3.52	20 (51%)
2	C47	C	1327	-	35,36,36	3.14	18 (51%)	39,50,50	2.98	17 (43%)

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
2	C47	O	1327	-	-	7/37/49/49	0/2/2/2
2	C47	C	1327	-	-	6/37/49/49	0/2/2/2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1327	C47	O4-C3	11.91	1.51	1.21
2	O	1327	C47	C12-C7	-8.19	1.28	1.40
2	C	1327	C47	C11-C12	7.99	1.52	1.39
2	C	1327	C47	C9-C8	7.82	1.52	1.38
2	O	1327	C47	C12-N13	7.71	1.54	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1327	C47	O2-C3-C5	9.02	125.25	111.76
2	O	1327	C47	C6-C5-C3	-7.51	86.70	110.40
2	C	1327	C47	O25-C24-C22	-6.95	96.28	109.48
2	O	1327	C47	O2-C3-O4	6.36	136.22	123.85
2	C	1327	C47	C28-C27-C29	6.35	121.30	109.64

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

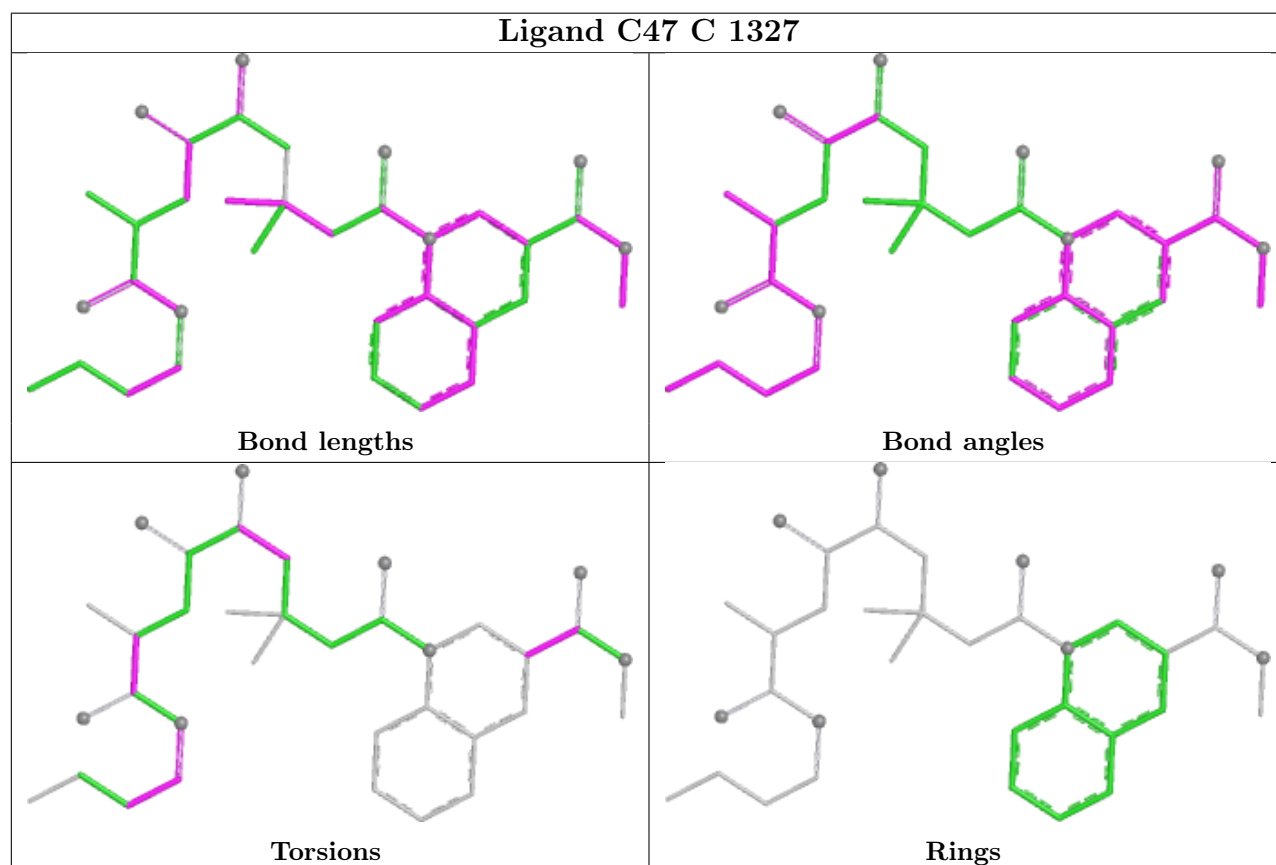
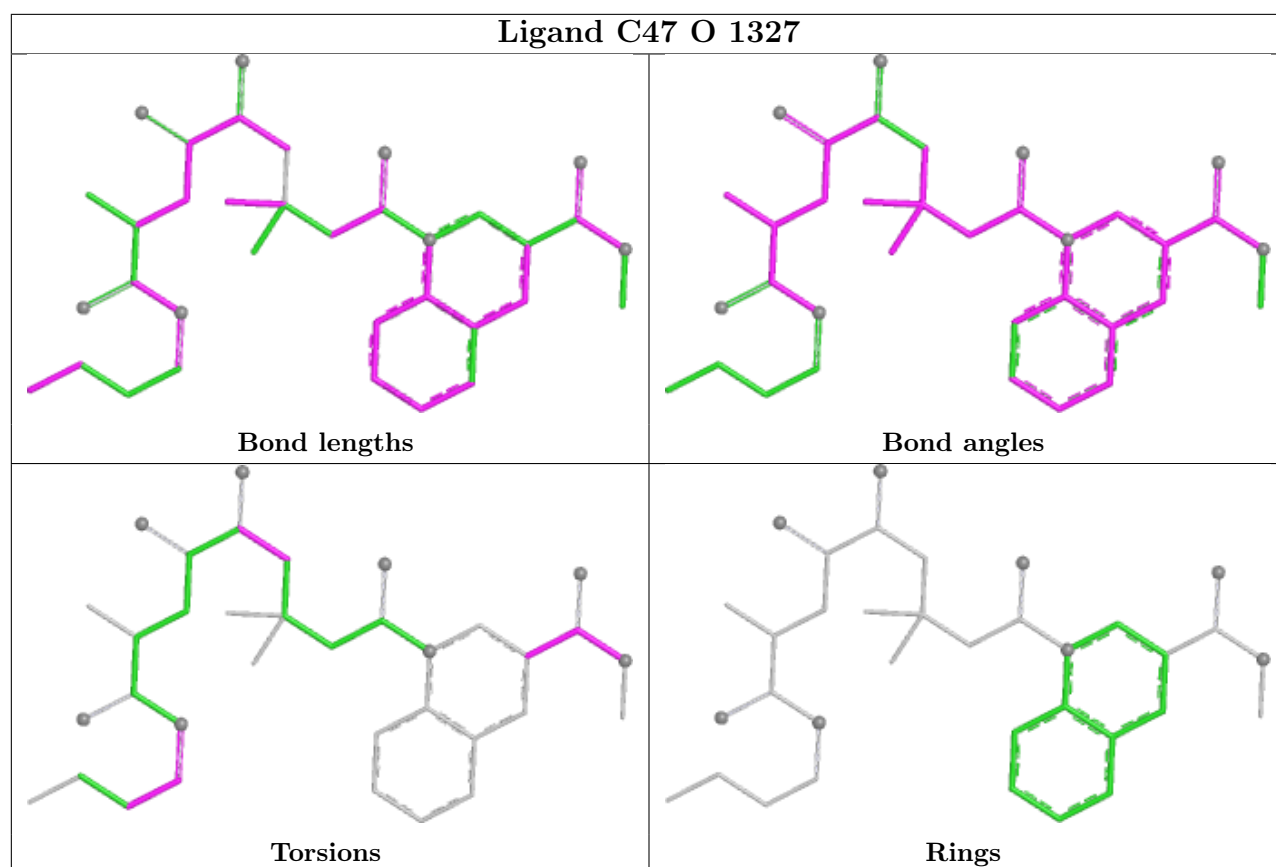
Mol	Chain	Res	Type	Atoms
2	C	1327	C47	C18-C21-C22-N23
2	C	1327	C47	C26-C27-C29-O30
2	O	1327	C47	O2-C3-C5-C14
2	O	1327	C47	O4-C3-C5-C14
2	O	1327	C47	C18-C21-C22-N23

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1327	C47	15	0
2	C	1327	C47	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	9
1	O	5

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	194:MET	C	195:LYS	N	1.20
1	O	258:ILE	C	259:SER	N	1.20
1	C	47:ARG	C	47(A):LEU	N	1.19
1	C	111:PRO	C	112:PHE	N	1.19
1	C	268:THR	C	269:LEU	N	1.19

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.