



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1QC9 / pdb_00001qc9
Title : THE CRYSTALLOGRAPHIC STRUCTURE OF RESTRICTION ENDONUCLEASE ECO RI AT 3.3 Å IN THE ABSENCE OF DNA
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Deposited on : 1999-05-18
Resolution : 3.00 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 ⓘ 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
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

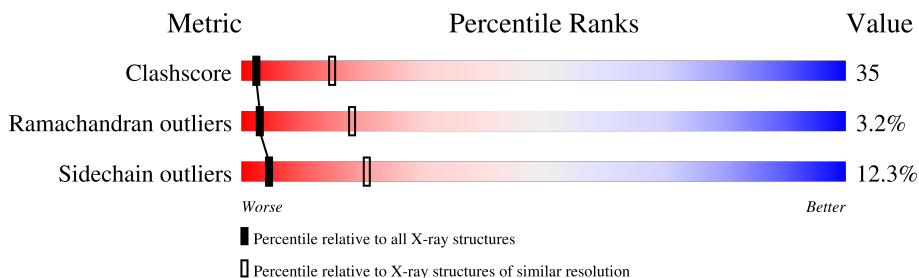
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	
1	B	276	
1	C	276	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5979 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 PROTEIN (ECO RI ENDONUCLEASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total 1993	C 1257	N 344	O 385	S 7	0	0	0
1	B	253	Total 1993	C 1257	N 344	O 385	S 7	0	0	0
1	C	253	Total 1993	C 1257	N 344	O 385	S 7	0	0	0



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.68Å 127.35Å 49.87Å 90.00° 98.57° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.251 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5979	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.78	5/2025 (0.2%)	1.11	11/2724 (0.4%)
1	B	0.77	5/2025 (0.2%)	1.11	11/2724 (0.4%)
1	C	0.78	5/2025 (0.2%)	1.11	11/2724 (0.4%)
All	All	0.78	15/6075 (0.2%)	1.11	33/8172 (0.4%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ARG	C-N	-8.88	1.21	1.33
1	B	145	ARG	C-N	-8.88	1.21	1.33
1	C	145	ARG	C-N	-8.87	1.21	1.33
1	A	19	GLY	N-CA	7.67	1.50	1.45
1	C	19	GLY	N-CA	7.63	1.50	1.45

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	GLY	N-CA-C	6.76	116.36	110.21
1	A	19	GLY	N-CA-C	6.76	116.36	110.21
1	B	19	GLY	N-CA-C	6.69	116.30	110.21
1	A	246	TRP	N-CA-C	6.33	119.39	109.96
1	C	246	TRP	N-CA-C	6.26	119.43	110.10

There are no chirality outliers.

There are no planarity outliers.

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	A	1993	0	1989	139	1
1	B	1993	0	1989	140	5
1	C	1993	0	1989	138	5
All	All	5979	0	5967	417	6

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 35.

The worst 5 of 417 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:A:183:ARG:CD	1:A:187:ARG:HB2	1.92	1.00
1:C:183:ARG:CD	1:C:187:ARG:HB2	1.92	0.99
1:B:183:ARG:CD	1:B:187:ARG:HB2	1.92	0.98
1:C:224:ASN:HD22	1:C:229:SER:HB3	1.30	0.95
1:B:136:LEU:HD11	1:B:138:ALA:HB3	1.50	0.94

The worst 5 of 6 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)
1:B:147:HIS:CB	1:C:144:GLU:O[2_555]	1.96	0.24
1:A:144:GLU:O	1:A:147:HIS:CB[2_555]	2.02	0.18
1:B:27:TYR:CD2	1:C:271:PHE:CE1[3_444]	2.02	0.18
1:B:27:TYR:CG	1:C:271:PHE:CE1[3_444]	2.12	0.08
1:B:27:TYR:CD2	1:C:271:PHE:CD1[3_444]	2.13	0.07

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	A	249/276 (90%)	209 (84%)	32 (13%)	8 (3%)	3 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	249/276 (90%)	209 (84%)	32 (13%)	8 (3%)	3	18
1	C	249/276 (90%)	209 (84%)	32 (13%)	8 (3%)	3	18
All	All	747/828 (90%)	627 (84%)	96 (13%)	24 (3%)	3	18

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	B	84	SER
1	C	84	SER
1	A	135	ASP
1	A	146	SER

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	
1	A	219/240 (91%)	192 (88%)	27 (12%)	4	21
1	B	219/240 (91%)	192 (88%)	27 (12%)	4	21
1	C	219/240 (91%)	192 (88%)	27 (12%)	4	21
All	All	657/720 (91%)	576 (88%)	81 (12%)	4	21

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	54	SER
1	C	187	ARG
1	C	62	LYS
1	C	136	LEU
1	C	205	THR

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	C	190	ASN
1	C	273	GLN
1	C	224	ASN
1	B	190	ASN
1	C	147	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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.