



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 07:37 PM EDT

PDB ID : 1SQ1 / pdb_00001sq1
Title : Crystal Structure of the Chorismate Synthase from *Campylobacter jejuni*,
Northeast Structural Genomics Target BR19
Authors : Forouhar, F.; Lee, I.; Vorobiev, S.M.; Xiao, R.; Acton, T.B.; Montelione, G.T.;
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Deposited on : 2004-03-17
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
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.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2168 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 Chorismate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	288	2151	1359	370	409	6	7	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9PM41
A	28	MSE	MET	modified residue	UNP Q9PM41
A	140	MSE	MET	modified residue	UNP Q9PM41
A	214	MSE	MET	modified residue	UNP Q9PM41
A	235	MSE	MET	modified residue	UNP Q9PM41
A	254	MSE	MET	modified residue	UNP Q9PM41
A	335	MSE	MET	modified residue	UNP Q9PM41
A	363	LEU	-	cloning artifact	UNP Q9PM41
A	364	GLU	-	cloning artifact	UNP Q9PM41
A	365	HIS	-	cloning artifact	UNP Q9PM41
A	366	HIS	-	cloning artifact	UNP Q9PM41
A	367	HIS	-	cloning artifact	UNP Q9PM41
A	368	HIS	-	cloning artifact	UNP Q9PM41
A	369	HIS	-	cloning artifact	UNP Q9PM41
A	370	HIS	-	cloning artifact	UNP Q9PM41

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	73.60Å 73.60Å 338.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.80	Depositor
% Data completeness (in resolution range)	9.5 (29.60-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.279	Depositor
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.897	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2168	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

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