



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:26 PM UTC

PDB ID : 2Q2E / pdb\_00002q2e  
Title : Crystal structure of the topoisomerase VI holoenzyme from *Methanosarcina mazei*  
Authors : Corbett, K.D.; Benedetti, P.; Berger, J.M.  
Deposited on : 2007-05-28  
Resolution : 4.00 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](mailto: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) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

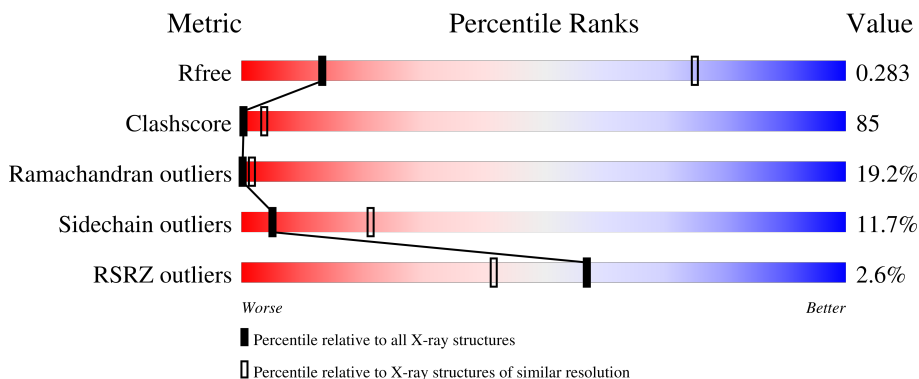
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	369	 3% 15% 46% 22% 15%
2	B	621	 2% 16% 49% 25% 6%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7039 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 Type II DNA topoisomerase VI subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2532	1610	423	490	9	0	0	0

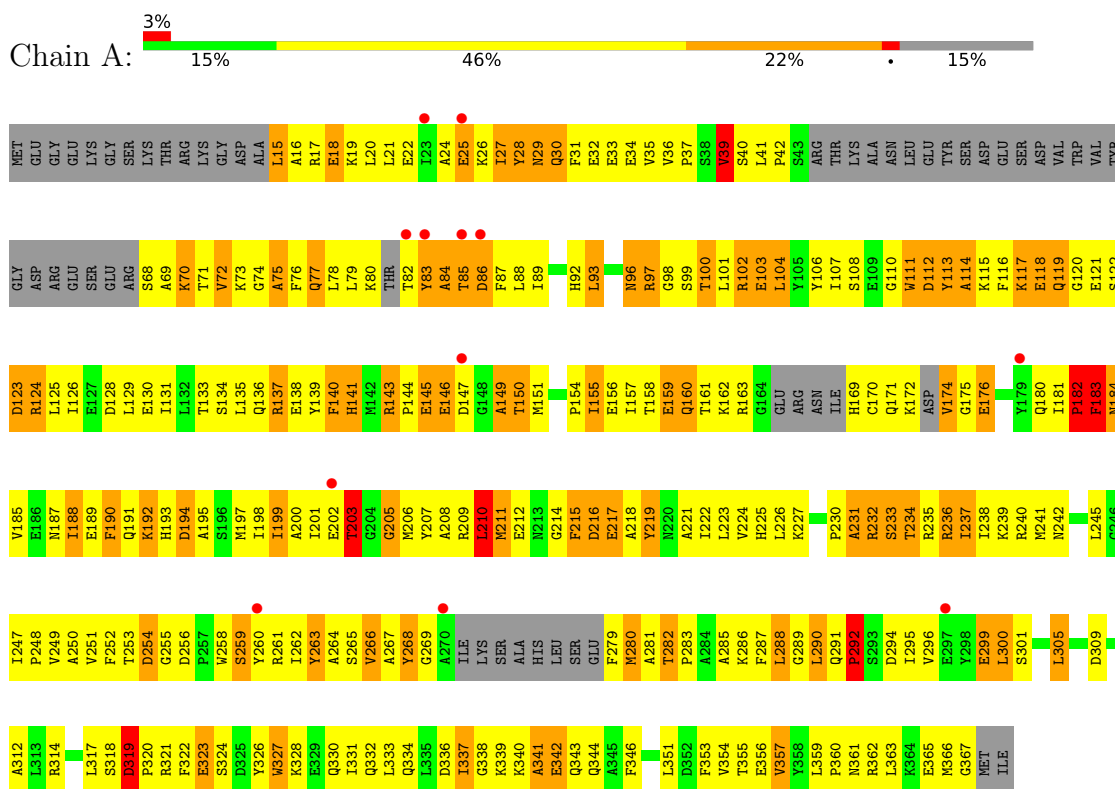
- Molecule 2 is a protein called Type 2 DNA topoisomerase 6 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	582	4507	2878	768	843	18	0	0	1

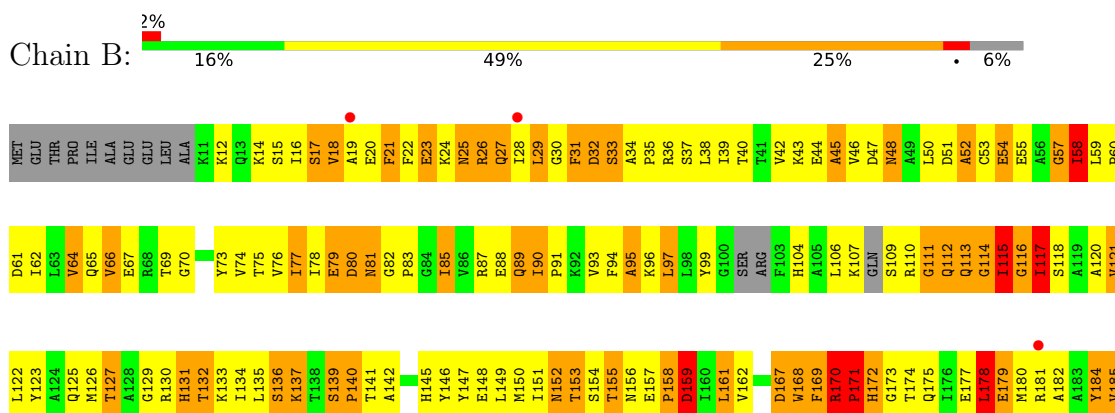
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Molecule 1: Type II DNA topoisomerase VI subunit A



- Molecule 2: Type 2 DNA topoisomerase 6 subunit B



E558	D497	A437	A377	L317	N249	K186
P559	V498	I438	N378	S318	L250	G187
K560	P499	A439	R379	P319	R251	R188
V562	D500	D440	V380	I320	R189	R189
T563	I501	I441	P381	G321	Q190	Q190
M564	N502	P442	L382	E322	S191	S191
	P503	V443	L383	D323	I192	I192
	V504	I444	Y384	L324	Y193	Y193
D567	V505	K445	Q385	I325	E194	E194
Y568	A506	E446	Q386	Y326	Y195	Y195
D569	K507	E447	G387	R327	ALA	L196
Y570	I508	I448	G388	G328	K197	K197
V571	M509	D449	C389	L329	A198	A198
	G510	L450	V390	E330	T199	T199
S575	M511	A451	T391	K331	A200	A200
A576	L512	L452	T392	E332	I201	I201
S577	L513	K453	H393	T333	V202	V202
	V514	E454	A394	T334	N203	N203
S580	H515	V455	V395	V335	P204	P204
K581	R516	A456	E396	D336	H205	H205
K582	V517	R457	D397	F337	A206	A206
V583	I518	K458	I398	I338	R207	R207
L584		L459	K399	A339	I208	I208
S585	N521	K460	N400	T340	T209	T209
Y586	G522	H461	K401	S341	L210	L210
K587	D523	Y462	Q402	T342	I211	I211
I588	G524	L463	Y403	R343	D212	D212
E589	T525	S464	G404	K344	P213	P213
S590	V526	K465	L405	P345	D214	D214
A591	D527	Q466	N406	A346	G215	G215
S592	V528	S467	Q407	Y347	N216	N216
E593	A529	M468	P408	Y348	E217	E217
E594	I530	L469	G409	S349	E218	E218
E595	K531	K470	G410	G350	V219	V219
L596	V532	K471	G411	I287	F220	F220
Q597	K533	R472	I412	D288	E221	E221
K598	M534	R473	P413	F353	R222	R222
L599	PHE	E474	V414	V354	A223	A223
P600	GLY	K475	G415	V355	T224	T224
Q601	THR	E476	P416	E356	D225	D225
L602	SER	I477	V417	V357	K226	K226
I603	A539	I478	I418	G358	N227	N227
V604	Y540	I479	L419	M359	P228	P228
E605	S541	T480	L420	A360	E229	E229
GLY	F542	K481	I421	Y361	P230	P230
ILE	R543	V482	H422	G362	A231	A231
GLU	V544	L483	V423	G363	E232	E232
GLU	H545	P484	A424	N364	E233	E233
GLU	E546	K485	S425	L365	I234	I234
LEU	M547	L486	T426	P366	L235	L235
VAL	L548	A487	M427	K367	P236	P236
T613	P549	A488	V428	E368	H237	H237
G614	C550	K489	P429	E369	P238	P238
A615	K551	V490	F430	K370	E239	E239
K616	V552	A491	T431	I371	G240	G240
ALA	SER	H492	S432	S372	I241	I241
PHE	GLY	V493	E433	I373	P313	P313
LYS	ALA	L494	S434	M374	T314	T314
GLY	K556	E495	K435	R375	D315	D315
VAL	P557	K496	D436	F376	C316	C316

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	227.81Å 227.81Å 208.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-4.00) 93.8 (30.00-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 4.01Å)	Xtrriage
Refinement program	REFMAC 5.3.0026	Depositor
R, $R_{free}$	0.306 , 0.349 0.301 , 0.283	Depositor DCC
$R_{free}$ test set	1298 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	153.1	Xtrriage
Anisotropy	0.370	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 213.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	192.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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	0.50	0/2579	1.13	25/3471 (0.7%)
2	B	0.67	0/4591	1.29	68/6215 (1.1%)
All	All	0.61	0/7170	1.24	93/9686 (1.0%)

There are no bond length outliers.

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	587	LYS	N-CA-C	11.59	123.52	108.34
2	B	223	ALA	N-CA-C	10.96	122.41	107.73
1	A	103	GLU	N-CA-C	-10.51	100.18	113.43
1	A	266	VAL	N-CA-C	-9.91	104.30	113.71
2	B	428	VAL	N-CA-C	9.86	119.34	107.61

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	2532	0	2476	415	0
2	B	4507	0	4565	808	0
All	All	7039	0	7041	1192	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 85.

The worst 5 of 1192 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:B:599:LEU:HD23	2:B:599:LEU:H	1.09	1.13
2:B:516:ARG:HH12	2:B:597:GLN:HB2	0.93	1.09
2:B:371:ILE:HG22	2:B:414:VAL:HG12	1.13	1.09
2:B:66:VAL:HG23	2:B:213:PRO:HD3	1.35	1.08
2:B:77:ILE:C	2:B:78:ILE:HD12	1.78	1.06

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	A	303/369 (82%)	163 (54%)	78 (26%)	62 (20%)	0	1
2	B	566/621 (91%)	339 (60%)	122 (22%)	105 (19%)	0	2
All	All	869/990 (88%)	502 (58%)	200 (23%)	167 (19%)	0	2

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	72	VAL
1	A	97	ARG
1	A	112	ASP
1	A	113	TYR

### 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	A	268/315 (85%)	239 (89%)	29 (11%)	6	24
2	B	486/527 (92%)	427 (88%)	59 (12%)	5	21
All	All	754/842 (90%)	666 (88%)	88 (12%)	5	21

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	214	ASP
2	B	397	ASP
2	B	218	GLU
2	B	357	VAL
2	B	436	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	152	ASN
2	B	378	ASN
2	B	502	ASN
2	B	406	ASN
1	A	193	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	315/369 (85%)	0.33	12 (3%) 44 34	139, 217, 258, 265	0
2	B	582/621 (93%)	0.10	11 (1%) 66 49	93, 175, 248, 265	0
All	All	897/990 (90%)	0.18	23 (2%) 57 42	93, 192, 254, 265	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	594	GLU	3.6
2	B	515	HIS	3.4
1	A	179	TYR	3.0
1	A	25	GLU	2.9
1	A	82	THR	2.7

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.