



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:56 PM GMT

PDB ID : 2Q2E
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 validation summary 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/ValidationPDFNotes.html>

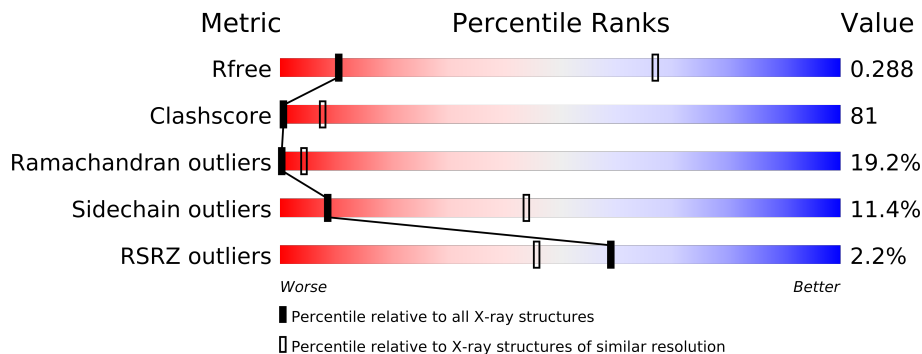
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	369	
2	B	621	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7039 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	315	Total	C	N	O	S	0	0	0
			2532	1610	423	490	9			

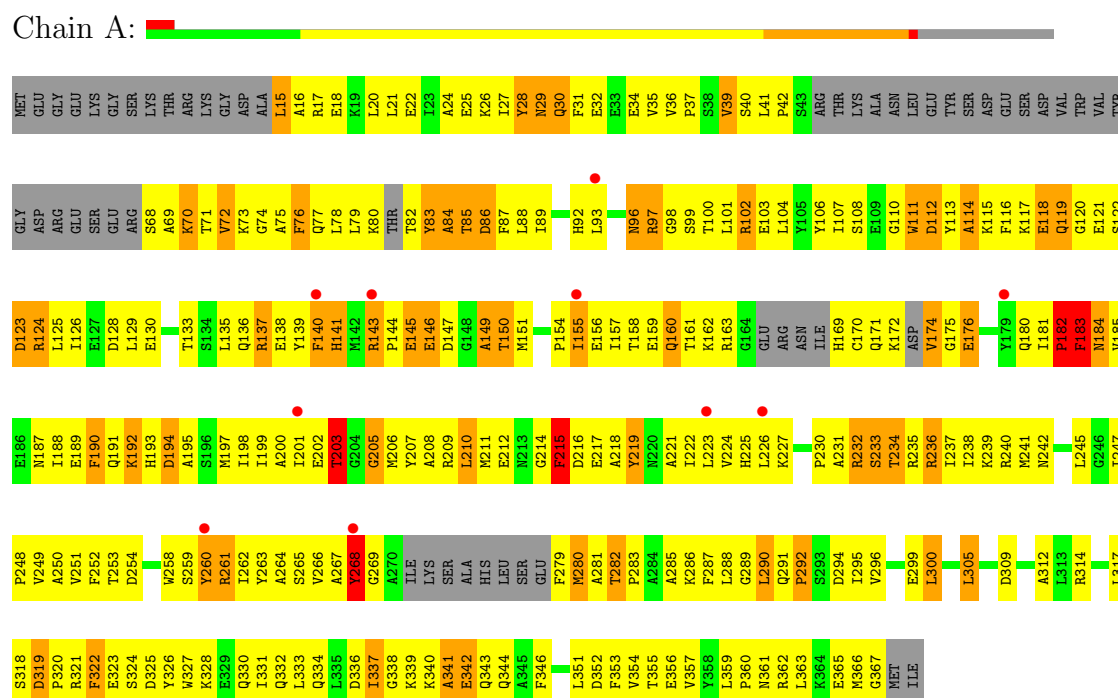
- Molecule 2 is a protein called Type 2 DNA topoisomerase 6 subunit B.

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

3 Residue-property plots

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.

• Molecule 1: Type II DNA topoisomerase VI subunit A



• Molecule 2: Type 2 DNA topoisomerase 6 subunit B



P559	K560	V561	M564	D567	Y568	D569	Y570	V571	S575	A576	S577	S580	S581	K582	Y583	L584	S585	Y586	K587	I588	E589	S590	A591	S592	S593	E594	E595	L596	Q597	K598	L599	P600	Q601	L602	I603	V604	GLY	ILE	GLY	GLU	GLU	GLU	LEU	VAL	T613	G614	A615	K616	ALA	PHE	LYS	GLY	VAL							
V498	P499	D500	I501	N502	P503	V504	V505	A506	K507	I508	M509	G510	G511	N511	L512	L513	V514	H515	R516	V517	L518	N521	G522	D523	G524	T525	V526	D527	V528	A529	I530	K531	V532	K533	N534	PHE	GLY	THR	SER	A539	Y540	S541	F542	R543	V544	H545	E546	M547	L548	P549	C550	K551	V552	SER	GLY	ALA	K556	P557	E558	
I438	A439	D440	I441	P442	V443	I444	K445	E446	E447	I448	D449	L450	A451	I452	K453	E454	V455	A456	R457	K458	L459	K460	H461	Y462	L463	S464	K465	Q466	S467	N468	L469	K470	R471	R472	R473	E474	K475	E476	I477	I478	I479	L480	K481	V482	L483	P484	K485	L486	A487	A488	K489	V490	A491	H492	V493	L494	E495	K496	D497	
N378	R379	V380	P381	L382	L383	Y384	Q385	Q386	Y387	G388	C389	V390	T391	T392	H393	A394	V395	D396	D397	I398	K399	W400	K401	Q402	Y403	G404	L405	N406	Q407	P408	G409	G410	G411	I412	F413	V414	G415	P416	V417	I418	L419	L420	I421	H422	V423	A424	N425	I426	N427	V428	P429	F430	T431	S432	E433	S434	K435	D436	A437	
S318	F319	I320	G321	E322	D323	L324	I325	Y326	R327	G328	L329	E330	K331	E332	T333	T334	V335	D336	F337	I338	A339	T340	S341	T342	R343	F344	L345	A346	V347	Y348	S349	G350	N351	P352	F353	V354	V355	E356	V357	G358	N359	A360	Y361	E362	G363	N364	L365	S425	P366	K367	E368	E369	K370	I371	S372	I373	K374	R375	F376	A377
Y252	T253	E254	ARG	GLN	LYS	LEU	ALA	P260	F261	L262	R263	C267	K268	ILE	GLY	L271	L272	T273	A274	I277	C278	A281	G282	L283	D284	P285	E286	I287	D288	P289	H290	A291	L292	G293	R294	A297	L300	L301	E302	A303	F304	E305	K306	V307	K308	I309	K310	A311	P312	T314	D315	C316	L317							

4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	227.81Å 227.81Å 208.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.00 92.23 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-4.00) 94.1 (92.23-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.306 , 0.349 0.306 , 0.288	Depositor DCC
R_{free} test set	1298 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	153.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 205.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 25919 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.41	0/2579	0.71	0/3471
2	B	0.51	1/4591 (0.0%)	0.83	5/6215 (0.1%)
All	All	0.47	1/7170 (0.0%)	0.79	5/9686 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	CYS	CB-SG	-6.66	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	GLY	N-CA-C	5.88	127.79	113.10
2	B	408	PRO	N-CA-CB	5.82	110.29	103.30
2	B	522	GLY	N-CA-C	-5.75	98.72	113.10
2	B	58	ILE	N-CA-C	5.66	126.29	111.00
2	B	362	GLY	N-CA-C	5.42	126.64	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2532	0	2476	393	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4507	0	4565	779	0
All	All	7039	0	7041	1140	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 81.

The worst 5 of 1140 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:599:LEU:H	2:B:599:LEU:HD23	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:222:ARG:HH21	2:B:332:GLU:HB2	1.12	1.06

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	
1	A	303/369 (82%)	163 (54%)	78 (26%)	62 (20%)	0	4
2	B	566/621 (91%)	339 (60%)	122 (22%)	105 (19%)	0	4
All	All	869/990 (88%)	502 (58%)	200 (23%)	167 (19%)	0	4

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 ⓘ

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%)	240 (90%)	28 (10%)	10	49
2	B	486/527 (92%)	428 (88%)	58 (12%)	8	42
All	All	754/842 (90%)	668 (89%)	86 (11%)	8	44

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	109	SER
2	B	171	PRO
2	B	540	TYR
2	B	117	ILE
2	B	159	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	48	ASN
2	B	190	GLN
1	A	344	GLN
2	B	378	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	315/369 (85%)	0.44	10 (3%) 45 36	139, 217, 258, 265	0
2	B	582/621 (93%)	0.40	10 (1%) 67 53	93, 175, 248, 265	0
All	All	897/990 (90%)	0.41	20 (2%) 59 46	93, 192, 254, 265	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	TYR	3.3
2	B	359	MET	3.2
1	A	226	LEU	3.0
1	A	143	ARG	2.9
2	B	294	ARG	2.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.