



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:14 PM GMT

PDB ID : 1W6T
Title : CRYSTAL STRUCTURE OF OCTAMERIC ENOLASE FROM STREPTOCOCCUS PNEUMONIAE
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Deposited on : 2004-08-24
Resolution : 2.10 Å(reported)

This is a full wwPDB validation 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>

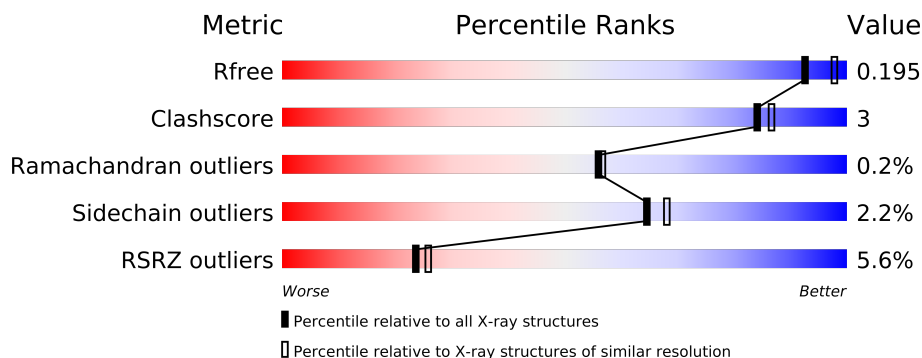
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	444	
1	B	444	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7393 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.

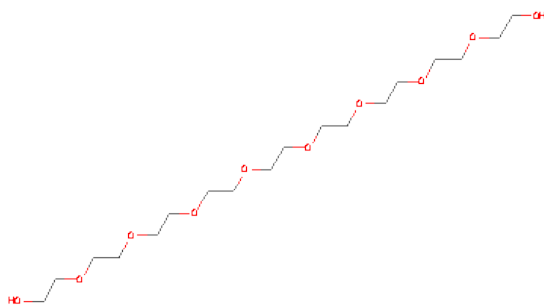
- Molecule 1 is a protein called ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	11	1
			3373	2122	573	669	9			
1	B	431	Total	C	N	O	S	0	19	1
			3457	2164	583	701	9			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 9	C 6	O 3	0	0
3	B	1	Total 17	C 11	O 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	276	Total 276	O 276	0	0
4	B	259	Total 259	O 259	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	143.70Å 143.70Å 100.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.10 19.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-2.10) 99.9 (19.93-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.148 , 0.187 0.161 , 0.195	Depositor DCC
R_{free} test set	3008 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 59527 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7393	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2PE

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	0.96	3/3429 (0.1%)	0.94	9/4633 (0.2%)
1	B	0.95	2/3511 (0.1%)	0.92	6/4745 (0.1%)
All	All	0.95	5/6940 (0.1%)	0.93	15/9378 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	CYS	CB-SG	-5.68	1.72	1.81
1	A	334	GLU	CG-CD	-5.38	1.43	1.51
1	A	8	TYR	CD1-CE1	5.36	1.47	1.39
1	B	77[A]	GLU	CG-CD	5.17	1.59	1.51
1	B	77[B]	GLU	CG-CD	5.17	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	308	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	253	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	308	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	180	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	85	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	146	MET	CG-SD-CE	6.21	110.14	100.20
1	B	308	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	372	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	14	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	58	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	120	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	120	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	58	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ASP	CB-CG-OD1	5.01	122.81	118.30

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	3373	0	3296	20	0
1	B	3457	0	3342	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	9	0	11	0	0
3	B	17	0	21	0	0
4	A	276	0	0	6	0
4	B	259	0	0	0	0
All	All	7393	0	6670	39	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 3.

All (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:157[B]:ASP:HB3	1:B:211[B]:ARG:NH2	1.88	0.88
1:B:157[B]:ASP:HB3	1:B:211[B]:ARG:HH21	1.56	0.70
1:A:24:GLU:OE1	4:A:2028:HOH:O	2.12	0.67
1:A:131:TYR:OH	1:A:416[B]:GLN:NE2	2.32	0.61
1:A:40:GLY:HA3	1:A:345:ASN:HD21	1.65	0.61
1:B:157[B]:ASP:CB	1:B:211[B]:ARG:NH2	2.62	0.60
1:A:294:MET:HG2	1:A:305:LEU:HD22	1.84	0.59
1:A:312[A]:LYS:NZ	4:A:2211:HOH:O	2.34	0.59
1:A:148[A]:ASN:O	1:A:397:SER:HB2	2.03	0.58
1:B:276:ASP:OD1	1:B:308:ARG:NH2	2.40	0.55
1:A:49:VAL:HG22	1:A:104:GLY:HA2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148[A]:ASN:HD21	1:A:151:ASN:HD21	1.55	0.54
1:A:294:MET:HE2	1:A:305:LEU:HD22	1.92	0.52
1:A:40:GLY:HA3	1:A:345:ASN:ND2	2.24	0.52
1:B:148[A]:ASN:O	1:B:397:SER:HB2	2.11	0.51
1:B:1:MET:HB3	1:B:29:SER:HB3	1.92	0.51
1:B:242:ASP:HA	1:B:291:GLU:HB3	1.93	0.50
1:B:299:TRP:CH2	1:B:330[A]:ARG:HD2	2.47	0.50
1:A:187:HIS:O	1:A:191[B]:LYS:HD2	2.13	0.48
1:B:294:MET:HG2	1:B:305:LEU:HD22	1.96	0.47
1:A:276:ASP:OD1	1:A:308:ARG:NH2	2.48	0.47
1:B:330[B]:ARG:O	1:B:334[B]:GLU:HG2	2.15	0.46
1:B:157[B]:ASP:CB	1:B:211[B]:ARG:HH21	2.27	0.46
1:B:150:ILE:HD11	1:B:189:LEU:HD21	1.98	0.46
1:B:294:MET:HE3	1:B:305:LEU:HB2	1.98	0.46
1:A:48:ALA:HB1	1:A:108:ALA:HB2	1.98	0.45
1:B:253:ARG:HH11	1:B:253:ARG:HG3	1.82	0.45
1:A:199:GLU:HG3	4:A:2167:HOH:O	2.18	0.44
1:B:191:LYS:HE2	1:B:191:LYS:HA	1.99	0.44
1:A:26[A]:TYR:OH	4:A:2028:HOH:O	2.21	0.43
1:A:312[B]:LYS:HD3	1:A:312[B]:LYS:O	2.18	0.43
1:B:49[B]:VAL:HG13	1:B:104:GLY:HA2	2.01	0.43
1:A:66:LYS:NZ	4:A:2071:HOH:O	2.53	0.42
1:A:191[B]:LYS:HD3	4:A:2160:HOH:O	2.19	0.42
1:A:1:MET:HB3	1:A:29:SER:HB3	2.02	0.42
1:B:294:MET:CE	1:B:305:LEU:HD22	2.50	0.41
1:B:48:ALA:HB1	1:B:108:ALA:HB2	2.02	0.41
1:A:187:HIS:HE1	1:B:16:ARG:O	2.04	0.41
1:B:278:LEU:HD12	1:B:294:MET:HE2	2.01	0.41

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	433/444 (98%)	420 (97%)	12 (3%)	1 (0%)	56 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	446/444 (100%)	433 (97%)	12 (3%)	1 (0%)	56	57
All	All	879/888 (99%)	853 (97%)	24 (3%)	2 (0%)	56	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
1	B	400	ARG

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	348/351 (99%)	338 (97%)	10 (3%)	55	57
1	B	358/351 (102%)	349 (98%)	9 (2%)	60	63
All	All	706/702 (101%)	687 (97%)	19 (3%)	64	60

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	140	LYS
1	A	155[A]	HIS
1	A	155[B]	HIS
1	A	199	GLU
1	A	264	GLU
1	A	312[A]	LYS
1	A	312[B]	LYS
1	A	371	HIS
1	A	402	ASP
1	B	45	GLU
1	B	77[A]	GLU
1	B	77[B]	GLU
1	B	102[A]	ASN
1	B	102[B]	ASN
1	B	253	ARG

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Mol	Chain	Res	Type
1	B	312	LYS
1	B	371	HIS
1	B	402	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	B	73	ASN
1	B	151	ASN
1	B	155	HIS
1	B	163	GLN
1	B	333	GLN

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
3	2PE	A	1434	-	8,8,27	1.01	1 (12%)	6,7,26	0.51	0
3	2PE	B	1434	-	15,16,27	0.71	0	14,15,26	0.53	0

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
3	2PE	A	1434	-	-	0/6/6/25	0/0/0/0
3	2PE	B	1434	-	-	0/14/14/25	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1434	2PE	C9-C8	-2.47	1.54	1.55

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	429/444 (96%)	0.08	30 (6%) 16 18	15, 21, 39, 64	0
1	B	431/444 (97%)	0.04	18 (4%) 35 39	15, 22, 39, 60	0
All	All	860/888 (96%)	0.06	48 (5%) 24 26	15, 21, 39, 64	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ALA	6.1
1	A	266	ALA	4.9
1	A	264	GLU	4.7
1	B	46	HIS	4.7
1	A	45	GLU	4.5
1	A	272	ALA	4.2
1	A	46	HIS	3.9
1	B	45	GLU	3.9
1	A	250	ASP	3.8
1	A	270	THR	3.7
1	B	252	GLU	3.6
1	A	268	VAL	3.4
1	B	251	LYS	3.4
1	A	155[A]	HIS	3.4
1	B	213[A]	GLU	3.3
1	A	253	ARG	3.3
1	B	263	GLY	3.2
1	B	264	GLU	3.2
1	A	267	ALA	3.0
1	B	159	PRO	2.9
1	A	263	GLY	2.8
1	B	253	ARG	2.8
1	A	255	VAL	2.7
1	A	0[A]	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	276	ASP	2.7
1	A	311	LYS	2.7
1	A	260	LYS	2.6
1	A	307	GLU	2.6
1	A	257	ASP	2.5
1	B	300	ASP	2.5
1	A	265	GLY	2.5
1	B	283[A]	ASN	2.5
1	A	254	LYS	2.4
1	A	157	ASP	2.4
1	A	273	GLU	2.4
1	A	275	ILE	2.4
1	B	265	GLY	2.4
1	A	249	TYR	2.4
1	A	259	THR	2.3
1	B	270	THR	2.3
1	B	254	LYS	2.2
1	A	246	SER	2.2
1	A	261	PHE	2.2
1	A	300	ASP	2.2
1	B	211[A]	ARG	2.1
1	B	0	HIS	2.0
1	A	213	GLU	2.0
1	B	54	GLY	2.0

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	2PE	B	1434	17/28	0.26	1.72	66,71,78,80	0
3	2PE	A	1434	9/28	0.17	1.17	69,71,76,76	0
2	MG	A	435	1/1	0.09	-1.52	32,32,32,32	0
2	MG	B	435	1/1	0.07	-1.66	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.