



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 07:50 AM EDT

PDB ID : 4EWJ
Title : structure of the enloase from Streptococcus suis serotype 2
Authors : Lu, Q.; Lu, H.; Qi, J.; Lu, G.; Gao, G.F.
Deposited on : 2012-04-27
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467
Xtrriage (Phenix) : 1.20.1
EDS : 2.36.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

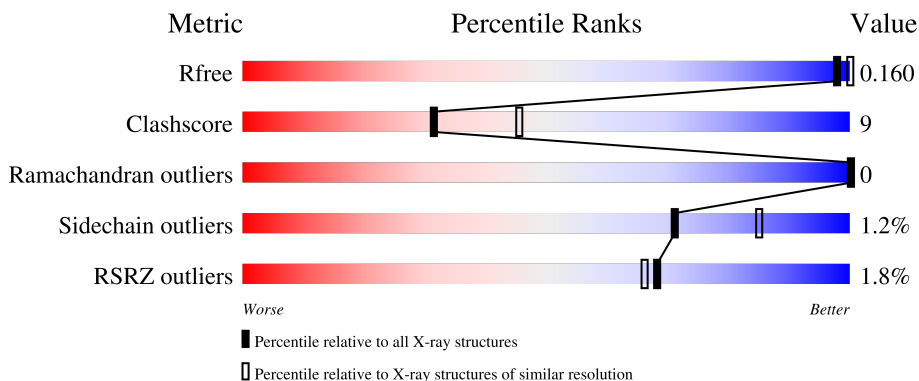
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


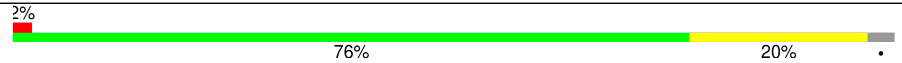
The reported resolution of this entry is 2.40 Å.

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	443	
1	B	443	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6751 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 Enolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	428	3257	2051	545	651	10	0	0	0
1	B	428	3260	2053	546	651	10	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	LEU	-	expression tag	UNP F4EGM3
A	437	GLU	-	expression tag	UNP F4EGM3
A	438	HIS	-	expression tag	UNP F4EGM3
A	439	HIS	-	expression tag	UNP F4EGM3
A	440	HIS	-	expression tag	UNP F4EGM3
A	441	HIS	-	expression tag	UNP F4EGM3
A	442	HIS	-	expression tag	UNP F4EGM3
A	443	HIS	-	expression tag	UNP F4EGM3
B	436	LEU	-	expression tag	UNP F4EGM3
B	437	GLU	-	expression tag	UNP F4EGM3
B	438	HIS	-	expression tag	UNP F4EGM3
B	439	HIS	-	expression tag	UNP F4EGM3
B	440	HIS	-	expression tag	UNP F4EGM3
B	441	HIS	-	expression tag	UNP F4EGM3
B	442	HIS	-	expression tag	UNP F4EGM3
B	443	HIS	-	expression tag	UNP F4EGM3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	119	Total	O	0	0
			119	119		
2	B	115	Total	O	0	0
			115	115		

4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	168.02Å 168.02Å 77.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.03 – 2.40 36.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (36.03-2.40) 98.1 (36.03-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.91 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.139 , 0.162 0.140 , 0.160	Depositor DCC
R_{free} test set	2077 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 20.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	0.450 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6751	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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.

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	0.21	0/3308	0.39	0/4474
1	B	0.21	0/3311	0.39	1/4477 (0.0%)
All	All	0.21	0/6619	0.39	1/8951 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	LYS	N-CA-CB	-5.21	101.22	110.60

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	3257	0	3185	64	0
1	B	3260	0	3194	53	0
2	A	119	0	0	3	0
2	B	115	0	0	2	0
All	All	6751	0	6379	116	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 9.

All (116) 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:236:ASN:N	1:A:237:GLY:HA2	1.78	0.97
1:B:236:ASN:N	1:B:237:GLY:HA2	1.78	0.97
1:B:171:GLY:HA3	1:B:236:ASN:HA	1.59	0.85
1:A:1:MET:HB3	1:A:29:SER:HB3	1.62	0.80
1:B:164:GLU:HB2	1:B:243:ASP:HB3	1.68	0.75
1:A:237:GLY:H	1:A:238:ILE:HA	1.52	0.74
1:A:304:LYS:HE2	1:A:335:GLU:HB3	1.70	0.72
1:A:232:GLU:HG2	1:A:233:ALA:H	1.55	0.71
1:A:206:GLY:HA3	2:A:591:HOH:O	1.90	0.71
1:A:79:ILE:HD12	1:A:90:ILE:HG23	1.74	0.70
1:A:164:GLU:HB2	1:A:243:ASP:HB3	1.72	0.70
1:A:171:GLY:HA3	1:A:236:ASN:HA	1.74	0.69
1:A:313:ARG:HG2	1:A:313:ARG:O	1.93	0.68
1:B:236:ASN:N	1:B:237:GLY:CA	2.54	0.68
1:A:163:GLN:HG2	1:A:164:GLU:HG3	1.76	0.68
1:B:79:ILE:HD12	1:B:90:ILE:HG23	1.78	0.66
1:B:56:LYS:HA	1:B:61:GLY:N	2.11	0.64
1:B:181:TRP:HZ3	1:B:236:ASN:O	1.81	0.63
1:B:1:MET:HB3	1:B:29:SER:HB3	1.80	0.62
1:A:236:ASN:N	1:A:237:GLY:CA	2.61	0.61
1:A:102:ASN:HB3	2:A:582:HOH:O	2.02	0.59
1:B:231:TYR:HA	2:B:570:HOH:O	2.04	0.58
1:A:237:GLY:N	1:A:238:ILE:HA	2.13	0.57
1:B:242:PHE:CE2	1:B:288:ILE:HD13	2.41	0.56
1:A:403:ASP:HB3	1:B:402:THR:OG1	2.05	0.56
1:A:103:LYS:HD3	1:A:111:ILE:HD12	1.88	0.56
1:A:259:TYR:HB2	1:A:268:ALA:O	2.07	0.55
1:B:234:GLY:HA2	1:B:239:MET:HG2	1.88	0.55
1:B:236:ASN:H	1:B:237:GLY:HA2	1.71	0.55
1:B:146:MET:HA	1:B:168:LEU:HG	1.89	0.54
1:A:342:LEU:HG	1:A:371:SER:HB2	1.88	0.54
1:A:181:TRP:HZ3	1:A:236:ASN:O	1.88	0.54
1:A:222:ILE:O	1:A:226:ILE:HG13	2.08	0.54
1:A:251:ASP:HB3	1:A:256:VAL:HG23	1.90	0.52
1:A:400:SER:O	1:A:401:ARG:HG3	2.09	0.52
1:B:295:MET:HG2	1:B:306:LEU:HD22	1.91	0.52
1:A:242:PHE:CE2	1:A:288:ILE:HD13	2.43	0.52
1:B:67:ALA:HB1	1:B:110:ALA:HB2	1.93	0.51
1:B:246:SER:HA	1:B:249:PHE:CE2	2.45	0.51
1:A:232:GLU:HB3	1:A:237:GLY:O	2.11	0.50
1:B:218:GLY:O	1:B:222:ILE:HG13	2.11	0.50
1:A:345:VAL:HG23	2:A:535:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:HG2	1:B:233:ALA:H	1.77	0.50
1:A:19:PRO:HG3	1:A:59:TYR:CG	2.47	0.50
1:A:425:LYS:HE3	1:A:429:SER:HA	1.94	0.49
1:B:296:ASP:HB3	1:B:299:ASP:HB2	1.94	0.49
1:B:272:SER:O	1:B:276:ILE:HG13	2.12	0.49
1:B:103:LYS:HE2	1:B:349:GLY:HA3	1.96	0.48
1:B:163:GLN:HG2	1:B:164:GLU:HG3	1.94	0.48
1:A:372:HIS:O	1:A:373:ARG:HD2	2.14	0.48
1:B:243:ASP:HA	1:B:292:GLU:HB3	1.96	0.48
1:A:60:LEU:HD11	2:B:525:HOH:O	2.14	0.48
1:B:300:TRP:CH2	1:B:331:ARG:HD3	2.49	0.48
1:A:209:ALA:N	1:A:210:PRO:HD3	2.30	0.47
1:B:279:LEU:O	1:B:283:VAL:HG23	2.15	0.47
1:B:304:LYS:O	1:B:308:GLU:HG3	2.14	0.47
1:B:194:LYS:HG3	1:B:200:THR:HG21	1.97	0.47
1:A:5:THR:HG21	1:A:28:GLU:HB2	1.97	0.47
1:B:180:ARG:NH2	1:B:181:TRP:HE1	2.12	0.47
1:A:372:HIS:ND1	1:A:404:ARG:NH1	2.62	0.46
1:B:12:VAL:HG23	1:B:20:THR:HG23	1.97	0.46
1:A:23:VAL:HG11	1:A:114:VAL:HG22	1.98	0.46
1:B:84:VAL:HG22	1:B:122:ALA:HB2	1.97	0.46
1:A:260:THR:HA	1:A:267:ALA:HB3	1.96	0.46
1:A:372:HIS:H	1:A:372:HIS:CD2	2.34	0.46
1:B:7:VAL:HG22	1:B:25:VAL:HG22	1.98	0.46
1:A:146:MET:HA	1:A:168:LEU:HG	1.98	0.45
1:B:24:GLU:HB3	1:B:32:PHE:HE1	1.81	0.45
1:B:237:GLY:H	1:B:238:ILE:HA	1.81	0.45
1:A:235:GLU:C	1:A:237:GLY:HA2	2.34	0.45
1:B:114:VAL:O	1:B:118:VAL:HG23	2.17	0.45
1:A:249:PHE:HB2	1:A:258:ASP:O	2.16	0.45
1:B:199:VAL:HG22	1:B:201:ALA:H	1.80	0.45
1:A:194:LYS:HG3	1:A:200:THR:HG21	1.99	0.44
1:B:56:LYS:HA	1:B:61:GLY:H	1.79	0.44
1:A:313:ARG:HD2	1:A:314:VAL:HG23	1.99	0.44
1:A:188:ALA:O	1:A:192:ILE:HG13	2.16	0.44
1:B:67:ALA:O	1:B:71:VAL:HG23	2.17	0.44
1:A:152:GLY:HA2	1:A:156:SER:HB3	2.00	0.44
1:A:37:VAL:HA	1:A:38:PRO:HD3	1.87	0.44
1:A:354:THR:O	1:A:358:ILE:HG13	2.17	0.44
1:A:329:LEU:O	1:A:333:ILE:HG13	2.18	0.44
1:B:53:ASP:HA	1:B:66:LYS:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ARG:HD2	1:B:314:VAL:HG23	2.00	0.44
1:B:9:ALA:HB2	1:B:23:VAL:HG22	2.00	0.43
1:A:141:VAL:HG11	1:A:425:LYS:HE2	1.99	0.43
1:A:382:ILE:HD11	1:A:407:LYS:HG2	2.00	0.43
1:B:209:ALA:N	1:B:210:PRO:HD3	2.32	0.43
1:B:387:VAL:HG21	1:B:414:ILE:HG21	1.99	0.43
1:A:149:ILE:HG23	1:A:150:ILE:HG12	2.00	0.43
1:B:88:GLN:O	1:B:92:ARG:HG2	2.19	0.43
1:A:112:LEU:HD22	1:A:346:ASN:HA	2.01	0.43
1:A:130:LEU:HD21	1:A:381:THR:HG23	1.99	0.43
1:B:237:GLY:N	1:B:238:ILE:HA	2.34	0.42
1:A:6:ASP:HB3	1:A:26:TYR:HB2	2.00	0.42
1:A:144:THR:HA	1:A:145:PRO:HD3	1.79	0.42
1:B:171:GLY:HA3	1:B:236:ASN:CA	2.41	0.42
1:A:272:SER:O	1:A:276:ILE:HG13	2.20	0.42
1:B:21:LEU:HD12	1:B:21:LEU:C	2.40	0.42
1:B:158:ALA:HB2	1:B:211:LYS:HA	2.01	0.42
1:B:409:ASN:O	1:B:413:ARG:HG3	2.19	0.42
1:A:21:LEU:HD12	1:A:21:LEU:C	2.40	0.42
1:B:2:SER:HB3	1:B:125:TYR:CZ	2.55	0.42
1:A:240:ILE:HG22	1:A:241:GLY:N	2.35	0.42
1:A:250:TYR:OH	1:A:255:LYS:HA	2.20	0.41
1:A:313:ARG:CD	1:A:314:VAL:HG23	2.50	0.41
1:A:27:THR:OG1	1:A:31:ALA:HB3	2.21	0.41
1:A:15:SER:HB3	1:A:403:ASP:HB3	2.03	0.41
1:A:88:GLN:O	1:A:92:ARG:HG2	2.20	0.41
1:A:218:GLY:O	1:A:222:ILE:HG13	2.21	0.41
1:A:258:ASP:OD1	1:A:269:VAL:HG22	2.21	0.41
1:A:410:GLN:O	1:A:414:ILE:HG13	2.20	0.41
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.95	0.41
1:A:74:VAL:HG12	1:A:97:LEU:HD21	2.03	0.40
1:B:60:LEU:HD12	1:B:60:LEU:N	2.36	0.40
1:B:345:VAL:HG23	1:B:346:ASN:N	2.36	0.40

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	422/443 (95%)	400 (95%)	22 (5%)	0	100	100
1	B	422/443 (95%)	401 (95%)	21 (5%)	0	100	100
All	All	844/886 (95%)	801 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	335/350 (96%)	331 (99%)	4 (1%)	71	85
1	B	336/350 (96%)	332 (99%)	4 (1%)	71	85
All	All	671/700 (96%)	663 (99%)	8 (1%)	71	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	313	ARG
1	A	372	HIS
1	A	403	ASP
1	B	77	ASP
1	B	372	HIS
1	B	403	ASP
1	B	428	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	428	ASN

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 monosaccharides 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, 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	428/443 (96%)	-0.32	7 (1%) 72 70	25, 37, 53, 77	0
1	B	428/443 (96%)	-0.28	8 (1%) 66 64	28, 38, 57, 83	0
All	All	856/886 (96%)	-0.30	15 (1%) 68 66	25, 38, 54, 83	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.5
1	B	1	MET	6.7
1	B	236	ASN	5.2
1	A	236	ASN	3.9
1	B	237	GLY	3.7
1	B	44	GLY	3.4
1	B	264	GLY	3.2
1	B	337	ALA	2.6
1	B	238	ILE	2.5
1	A	46	HIS	2.5
1	B	254	ARG	2.5
1	A	337	ALA	2.4
1	A	45	GLU	2.3
1	A	237	GLY	2.2
1	A	238	ILE	2.1

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 monosaccharides 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.