Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2024 – 02:50 PM JST

PDB ID	:	8JUO
Title	:	Crystal structure of aspartate semialdehyde dehydrogenase from Porphyromonas gingivalis
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Deposited on	:	2023-06-27
Resolution	:	1.73 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:

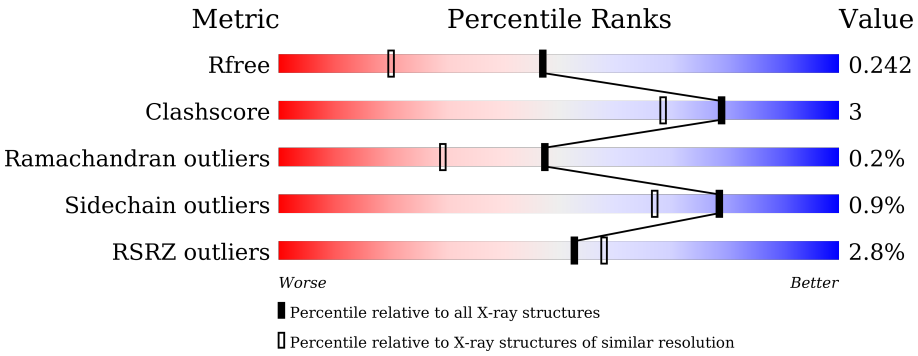
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 <=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	337	2% 91% 9%
1	B	337	4% 92% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5542 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 Aspartate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2598	1642	448	491	17			
1	B	335	Total	C	N	O	S	0	0	0
			2598	1642	448	491	17			

- Molecule 2 is water.

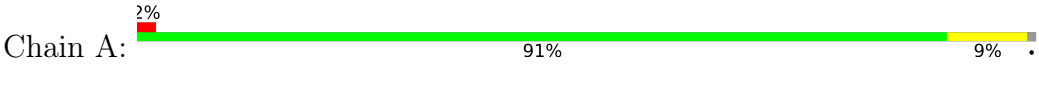
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	169	Total	O	0	0
			169	169		

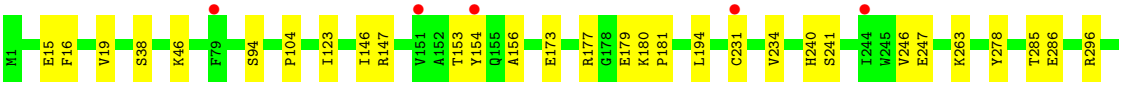
3 Residue-property plots (i)

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: Aspartate-semialdehyde dehydrogenase

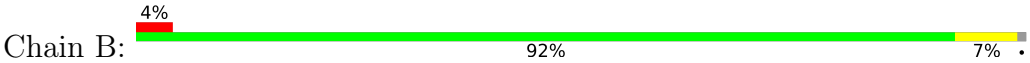
Chain A:

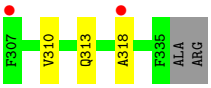




• Molecule 1: Aspartate-semialdehyde dehydrogenase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.86Å 108.86Å 162.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 1.73 29.75 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.75-1.73) 99.6 (29.75-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.5, PHENIX 1.14_3260	Depositor
R, R_{free}	0.216 , 0.238 0.224 , 0.242	Depositor DCC
R_{free} test set	3363 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5542	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5011e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.39	0/2649	0.59	1/3590 (0.0%)
1	B	0.43	0/2649	0.58	0/3590
All	All	0.41	0/5298	0.58	1/7180 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	ARG	NE-CZ-NH2	-5.96	117.32	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2598	0	2586	15	0
1	B	2598	0	2586	14	0
2	A	177	0	0	3	0
2	B	169	0	0	1	0
All	All	5542	0	5172	29	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 3.

All (29) 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:B:297:GLN:HG2	2:B:476:HOH:O	1.79	0.82
1:B:93:ASN:HD22	1:B:125:ASN:HD22	1.45	0.64
1:B:100:GLN:OE1	1:B:120:ARG:NH1	2.39	0.55
1:B:167:GLU:O	1:B:171:GLN:HG3	2.06	0.55
1:A:173:GLU:HG2	2:A:525:HOH:O	2.08	0.54
1:A:156:ALA:H	1:A:240:HIS:CE1	2.26	0.53
1:B:174:GLU:OE1	1:B:182:THR:OG1	2.27	0.52
1:A:177:ARG:HD2	1:A:179:GLU:OE1	2.11	0.50
1:A:153:THR:OG1	1:A:231:CYS:HA	2.13	0.48
1:A:104:PRO:HG2	1:A:123:ILE:HG12	1.95	0.48
1:A:263:LYS:HG3	2:A:472:HOH:O	2.14	0.47
1:A:15:GLU:O	1:A:19:VAL:HG12	2.14	0.46
1:A:154:TYR:HB2	1:A:241:SER:HB2	1.97	0.46
1:A:16:PHE:HA	1:A:19:VAL:HG12	1.97	0.46
1:B:244:ILE:HG22	1:B:246:VAL:HG23	1.96	0.46
1:B:93:ASN:ND2	1:B:125:ASN:HD22	2.13	0.45
1:A:146:ILE:HG23	1:A:246:VAL:CG1	2.47	0.45
1:B:240:HIS:NE2	1:B:313:GLN:HG3	2.31	0.44
1:B:153:THR:OG1	1:B:231:CYS:HA	2.18	0.43
1:A:46:LYS:HE2	2:A:430:HOH:O	2.19	0.43
1:A:285:THR:HG22	1:A:286:GLU:HG3	2.00	0.43
1:A:194:LEU:HD22	1:A:234:VAL:HG12	2.01	0.43
1:B:16:PHE:HA	1:B:19:VAL:HG12	2.01	0.43
1:A:147:ARG:NH1	1:A:247:GLU:OE1	2.52	0.43
1:A:180:LYS:HA	1:A:181:PRO:HD3	1.87	0.42
1:B:241:SER:OG	1:B:310:VAL:HG22	2.20	0.42
1:B:240:HIS:HE2	1:B:313:GLN:HG3	1.86	0.41
1:B:285:THR:HG22	1:B:286:GLU:HG3	2.02	0.41
1:B:146:ILE:HG23	1:B:246:VAL:HG13	2.02	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	333/337 (99%)	323 (97%)	10 (3%)	0	100 100
1	B	333/337 (99%)	320 (96%)	12 (4%)	1 (0%)	41 23
All	All	666/674 (99%)	643 (96%)	22 (3%)	1 (0%)	47 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	ALA

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	280/281 (100%)	277 (99%)	3 (1%)	73 59
1	B	280/281 (100%)	278 (99%)	2 (1%)	84 75
All	All	560/562 (100%)	555 (99%)	5 (1%)	78 67

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	94	SER
1	A	278	TYR
1	B	177	ARG
1	B	278	TYR

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	93	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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, 95^{th} 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	335/337 (99%)	0.13	6 (1%) 68 74	17, 26, 42, 59	0
1	B	335/337 (99%)	0.14	13 (3%) 39 45	19, 27, 43, 67	0
All	All	670/674 (99%)	0.13	19 (2%) 53 58	17, 26, 42, 67	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	TYR	4.6
1	B	154	TYR	4.6
1	B	177	ARG	3.6
1	B	74	ASP	2.9
1	A	244	ILE	2.8
1	B	152	ALA	2.7
1	A	308	TRP	2.6
1	A	231	CYS	2.5
1	B	91	ILE	2.3
1	B	81	ASP	2.3
1	B	128	CYS	2.3
1	A	79	PHE	2.2
1	B	307	PHE	2.2
1	B	175	LEU	2.2
1	A	151	VAL	2.1
1	B	68	PHE	2.1
1	B	151	VAL	2.1
1	B	28	ASP	2.1
1	B	318	ALA	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 (i)

There are no monosaccharides 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.