



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:02 pm BST

PDB ID : 5JAY
Title : Crystal Structure of an 8-amino-7-oxononanoate Synthase from Burkholderia xenovorans
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2016-04-12
Resolution : 1.75 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 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	:	2.11
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)	:	2.11

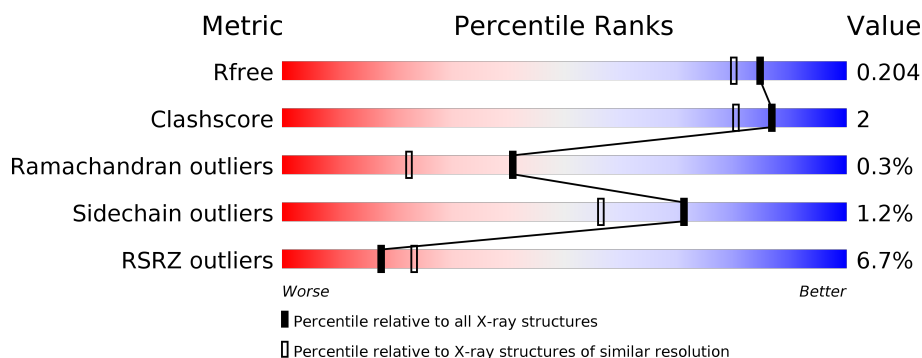
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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	402	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	402	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>.</div> <div>9%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5985 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 8-amino-7-oxononanoate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	3	0
			2776	1745	500	522	9			
1	B	364	Total	C	N	O	S	0	7	0
			2654	1661	482	504	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q146K3
A	-6	ALA	-	expression tag	UNP Q146K3
A	-5	HIS	-	expression tag	UNP Q146K3
A	-4	HIS	-	expression tag	UNP Q146K3
A	-3	HIS	-	expression tag	UNP Q146K3
A	-2	HIS	-	expression tag	UNP Q146K3
A	-1	HIS	-	expression tag	UNP Q146K3
A	0	HIS	-	expression tag	UNP Q146K3
A	241	ASP	GLY	engineered mutation	UNP Q146K3
B	-7	MET	-	initiating methionine	UNP Q146K3
B	-6	ALA	-	expression tag	UNP Q146K3
B	-5	HIS	-	expression tag	UNP Q146K3
B	-4	HIS	-	expression tag	UNP Q146K3
B	-3	HIS	-	expression tag	UNP Q146K3
B	-2	HIS	-	expression tag	UNP Q146K3
B	-1	HIS	-	expression tag	UNP Q146K3
B	0	HIS	-	expression tag	UNP Q146K3
B	241	ASP	GLY	engineered mutation	UNP Q146K3

- Molecule 2 is water.

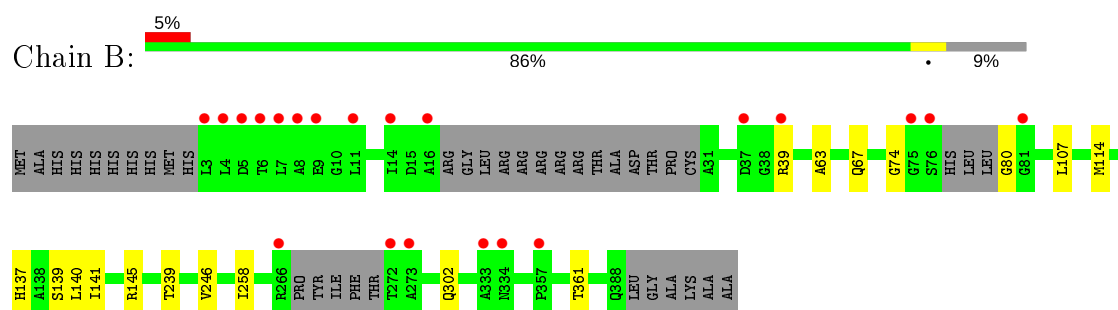
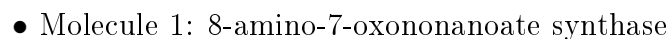
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	256	Total	O	0	6
			262	262		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	289	Total 293	O 293	0	4

- Molecule 1: 8-amino-7-oxononanoate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.87Å 63.20Å 65.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.41 – 1.75 43.87 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.41-1.75) 99.9 (43.87-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 1.75Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.171 , 0.204 0.172 , 0.204	Depositor DCC
R_{free} test set	1914 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5985	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

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	0.32	0/2837	0.49	0/3874
1	B	0.34	0/2720	0.54	0/3703
All	All	0.33	0/5557	0.51	0/7577

There are no bond length outliers.

There are no bond angle outliers.

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	2776	0	2702	14	0
1	B	2654	0	2604	9	0
2	A	262	0	0	5	0
2	B	293	0	0	1	0
All	All	5985	0	5306	22	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 2.

All (22) 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:137:HIS:CD2	1:A:139:SER:HB3	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:HG	1:B:258:ILE:HG23	1.80	0.63
1:A:102:GLU:OE2	1:A:230:ARG:NH2	2.35	0.57
1:A:118:ALA:HB2	1:A:269:ILE:HG21	1.88	0.56
1:A:137:HIS:CE1	1:A:140:LEU:HG	2.43	0.53
1:B:137[B]:HIS:CE1	1:B:140:LEU:HG	2.44	0.52
1:A:240:LEU:HD13	1:A:282:VAL:HG11	1.90	0.51
1:A:99:GLY:O	1:A:230:ARG:NH1	2.40	0.49
2:A:548[A]:HOH:O	1:B:114:MET:HG2	2.15	0.47
1:B:137[B]:HIS:CD2	1:B:139:SER:HG	2.34	0.46
1:A:350:TRP:CH2	1:B:80:GLY:HA3	2.50	0.46
1:B:141:ILE:O	1:B:145:ARG:HG2	2.16	0.46
1:A:107:LEU:HG	1:A:258:ILE:HG23	1.97	0.46
1:A:330:ILE:HD13	1:A:365:ARG:HB3	1.98	0.45
2:A:487:HOH:O	1:B:74:GLY:HA2	2.17	0.44
1:A:114:MET:HG2	2:A:548[B]:HOH:O	2.17	0.43
1:A:202:GLY:HA2	2:A:501:HOH:O	2.19	0.42
1:B:302:GLN:NE2	2:B:411:HOH:O	2.49	0.41
1:B:63:ALA:O	1:B:67:GLN:HG2	2.21	0.41
1:A:114:MET:SD	1:A:269:ILE:HG23	2.61	0.40
1:A:137:HIS:HD2	1:A:139:SER:HB3	1.83	0.40
1:A:302:GLN:NE2	2:A:403:HOH:O	2.35	0.40

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	384/402 (96%)	380 (99%)	3 (1%)	1 (0%)	41	22
1	B	363/402 (90%)	356 (98%)	6 (2%)	1 (0%)	41	22
All	All	747/804 (93%)	736 (98%)	9 (1%)	2 (0%)	41	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	VAL
1	B	246	VAL

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	264/295 (90%)	261 (99%)	3 (1%)	73	60
1	B	256/295 (87%)	253 (99%)	3 (1%)	71	56
All	All	520/590 (88%)	514 (99%)	6 (1%)	71	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	139	SER
1	A	272	THR
1	B	39	ARG
1	B	239	THR
1	B	361	THR

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

Mol	Chain	Res	Type
1	A	137	HIS

5.3.3 RNA ⓘ

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 carbohydrates 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 ⓘ

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	385/402 (95%)	0.30	29 (7%) 14 19	16, 28, 57, 71	0
1	B	364/402 (90%)	0.16	21 (5%) 23 28	13, 23, 57, 71	0
All	All	749/804 (93%)	0.23	50 (6%) 17 23	13, 26, 57, 71	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	6.2
1	B	4	LEU	5.2
1	A	16	ALA	5.2
1	B	8	ALA	4.9
1	B	6	THR	4.9
1	A	19	LEU	4.7
1	B	5	ASP	4.5
1	A	14	ILE	4.4
1	A	146	LEU	4.0
1	A	144	ALA	4.0
1	A	125	GLY	3.8
1	B	11	LEU	3.8
1	B	14	ILE	3.7
1	B	334	ASN	3.7
1	A	333	ALA	3.6
1	A	18	GLY	3.6
1	A	17	ARG	3.6
1	B	81	GLY	3.6
1	B	266	ARG	3.5
1	A	-2	HIS	3.4
1	A	357	PRO	3.3
1	A	126	ARG	3.2
1	A	82	HIS	3.1
1	A	147	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	16	ALA	2.9
1	A	260	TRP	2.9
1	A	173	VAL	2.9
1	A	141	ILE	2.9
1	B	37	ASP	2.9
1	B	9	GLU	2.9
1	B	75	GLY	2.8
1	B	7	LEU	2.6
1	A	361	THR	2.6
1	B	39	ARG	2.5
1	B	272	THR	2.5
1	B	76	SER	2.5
1	A	168	ALA	2.4
1	B	273	ALA	2.4
1	A	271	THR	2.3
1	A	15	ASP	2.3
1	A	389	LEU	2.2
1	A	262	VAL	2.2
1	B	357	PRO	2.1
1	A	153	ILE	2.1
1	B	333	ALA	2.1
1	A	10	GLY	2.1
1	A	201	HIS	2.1
1	A	256	THR	2.0
1	A	169	SER	2.0
1	A	11	LEU	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.