

wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2024 – 12:09 PM JST

PDB ID : 8JTU

Title: Connectase T1A mutant from Methanocaldococcus mazei

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Deposited on : 2023-06-22

Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.21 \end{array}$

EDS: 3.0

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.004 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

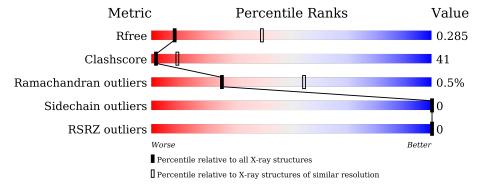
Validation Pipeline (wwPDB-VP) : 2.40

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 3.40 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	192	38%	60%	·		
1	В	192	38%	60%	•		



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2944 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 Connectase.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	Λ	192	Total	С	N	О	S	0	0	0	
1	Α		1472	921	253	288	10	U		U	
1	D	192	Total	С	N	О	S	0	0	0	
1	Ъ	192	1472	921	253	288	10	U		U	

There are 2 discrepancies between the modelled and reference sequences:

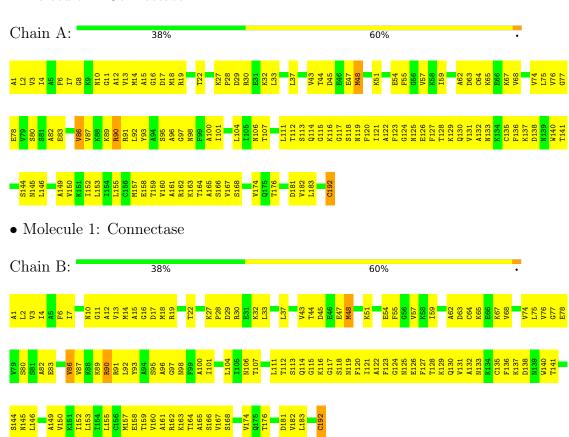
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP A0A0F8NKN3
В	1	ALA	-	expression tag	UNP A0A0F8NKN3



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: Connectase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	90.72Å 90.72Å 90.46Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.55 - 3.40	Depositor
Resolution (A)	40.55 - 3.40	EDS
% Data completeness	99.5 (40.55-3.40)	Depositor
(in resolution range)	99.8 (40.55-3.40)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.86 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
D D	0.207 , 0.288	Depositor
R, R_{free}	0.208 , 0.285	DCC
R_{free} test set	310 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	118.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 515.4	EDS
L-test for twinning ²	$< L >=0.42, < L^2>=0.24$	Xtriage
Estimated twinning fraction	0.418 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2944	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.77% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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		nd lengths	Bond angles		
WIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.86	1/1485 (0.1%)	1.20	3/1987 (0.2%)	
1	В	0.86	1/1485 (0.1%)	1.20	3/1987 (0.2%)	
All	All	0.86	$2/2970 \ (0.1\%)$	1.20	6/3974 (0.2%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	83	GLU	CB-CG	5.88	1.63	1.52
1	В	83	GLU	CB-CG	5.81	1.63	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	48	MET	CG-SD-CE	5.98	109.77	100.20
1	В	48	MET	CG-SD-CE	5.95	109.72	100.20
1	В	192	CYS	CA-CB-SG	5.08	123.15	114.00
1	A	90	ARG	CB-CG-CD	-5.08	98.40	111.60
1	В	90	ARG	CB-CG-CD	-5.08	98.40	111.60

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	1472	0	1507	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	1472	0	1507	121	0
All	All	2944	0	3014	242	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 41.

The worst 5 of 242 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mathring{\mathbf{A}}) \end{aligned}$
1:A:29:ASP:HA	1:A:32:LYS:HD2	1.37	1.04
1:B:29:ASP:HA	1:B:32:LYS:HD2	1.37	1.03
1:A:119:ASN:OD1	1:A:120:PHE:N	2.10	0.85
1:B:119:ASN:OD1	1:B:120:PHE:N	2.10	0.84
1:B:13:VAL:HG22	1:B:153:LEU:HD22	1.64	0.80

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	190/192 (99%)	168 (88%)	21 (11%)	1 (0%)	25	54	
1	В	190/192 (99%)	167 (88%)	22 (12%)	1 (0%)	25	54	
All	All	380/384 (99%)	335 (88%)	43 (11%)	2 (0%)	25	54	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	В	86	VAL



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	160/160 (100%)	160 (100%)	0	100	100
1	В	160/160 (100%)	160 (100%)	0	100	100
All	All	320/320 (100%)	320 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	В	175	GLN

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 oligosaccharides 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, 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 $>$	$\#\text{RSRZ}{>}2$		RZ>2	$OWAB(Å^2)$	Q<0.9
1	A	192/192~(100%)	-1.43	0	100	100	103, 219, 335, 434	0
1	В	192/192~(100%)	-1.45	0	100	100	103, 219, 335, 434	0
All	All	384/384 (100%)	-1.44	0	100	100	103, 219, 335, 434	0

There are no RSRZ outliers to report.

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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

