



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:41 PM UTC

PDB ID : 8SF5 / pdb_00008sf5
Title : Promiscuous amino acid gamma synthase from Caldicellulosiruptor hydrothermalis in open conformation
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Deposited on : 2023-04-10
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

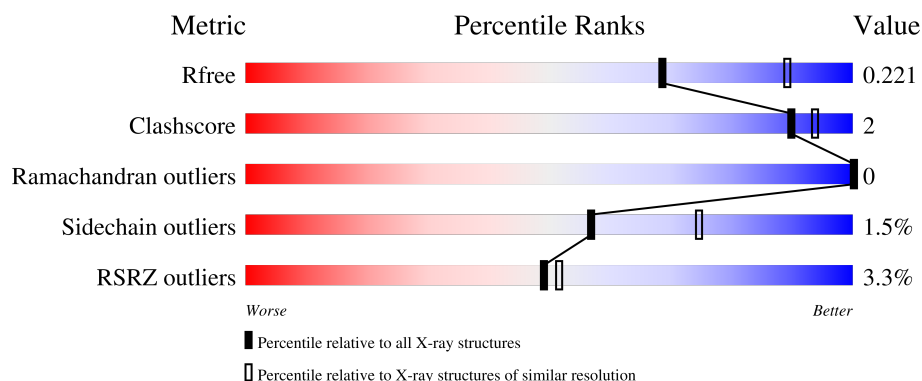
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

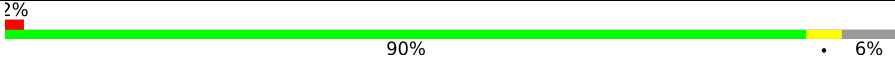
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	433	
1	B	433	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6191 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 O-acetylhomoserine/O-acetylserine sulfhydrylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	P	S	0	1	0
			3116	2013	512	584	1	6			
1	B	403	Total	C	N	O	P	S	0	1	0
			3045	1967	500	571	1	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	LEU	-	expression tag	UNP E4QC33
A	427	GLU	-	expression tag	UNP E4QC33
A	428	HIS	-	expression tag	UNP E4QC33
A	429	HIS	-	expression tag	UNP E4QC33
A	430	HIS	-	expression tag	UNP E4QC33
A	431	HIS	-	expression tag	UNP E4QC33
A	432	HIS	-	expression tag	UNP E4QC33
A	433	HIS	-	expression tag	UNP E4QC33
B	426	LEU	-	expression tag	UNP E4QC33
B	427	GLU	-	expression tag	UNP E4QC33
B	428	HIS	-	expression tag	UNP E4QC33
B	429	HIS	-	expression tag	UNP E4QC33
B	430	HIS	-	expression tag	UNP E4QC33
B	431	HIS	-	expression tag	UNP E4QC33
B	432	HIS	-	expression tag	UNP E4QC33
B	433	HIS	-	expression tag	UNP E4QC33

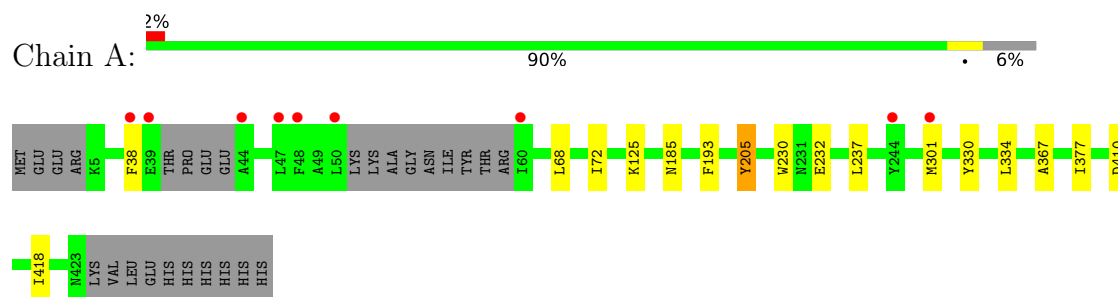
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total	O	0	0
			24	24		
2	B	6	Total	O	0	0
			6	6		

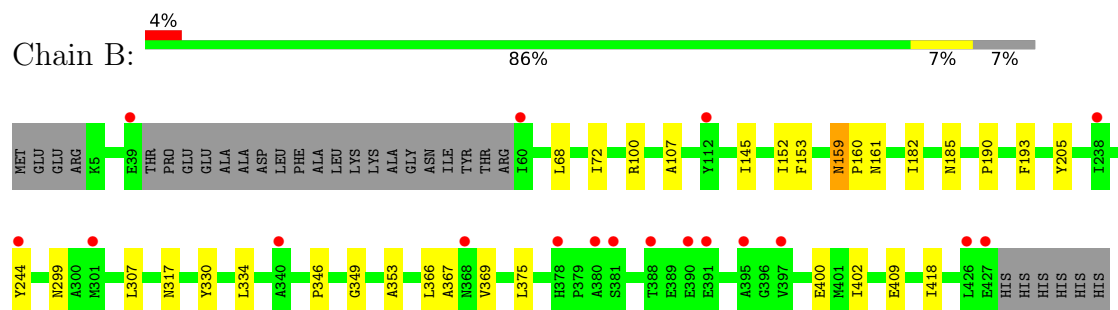
3 Residue-property plots [i](#)

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: O-acetylhomoserine/O-acetylserine sulfhydrylase



- Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.92Å 79.92Å 230.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.32 – 2.30 44.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.32-2.30) 99.9 (44.32-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.243 (Not available) , 0.221	Depositor DCC
R_{free} test set	2006 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6191	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	1.01	0/3162	1.39	0/4304
1	B	1.02	0/3091	1.42	2/4221 (0.0%)
All	All	1.02	0/6253	1.40	2/8525 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	349	GLY	CA-C-N	5.60	128.09	120.54
1	B	349	GLY	C-N-CA	5.60	128.09	120.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Peptide

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	3116	0	3043	8	0
1	B	3045	0	2925	16	0
2	A	24	0	0	0	0
2	B	6	0	0	0	0
All	All	6191	0	5968	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:B:307:LEU:HD21	1:B:418:ILE:HG21	1.81	0.62
1:A:193:PHE:HB2	1:A:334:LEU:CD2	2.42	0.50
1:A:38:PHE:HZ	1:B:367:ALA:HB2	1.77	0.49
1:A:68:LEU:O	1:A:72:ILE:HG12	2.15	0.47
1:A:367:ALA:HA	1:A:377:ILE:HD12	1.96	0.47
1:B:185:ASN:HB3	1:B:205:TYR:CE2	2.51	0.46
1:B:369:VAL:HA	1:B:375:LEU:HD12	1.97	0.46
1:B:161:ASN:O	1:B:317:ASN:ND2	2.43	0.46
1:B:159:ASN:HD22	1:B:159:ASN:HA	1.60	0.45
1:B:299:ASN:ND2	1:B:409:GLU:O	2.50	0.44
1:A:232:GLU:H	1:A:232:GLU:CD	2.26	0.44
1:B:68:LEU:O	1:B:72:ILE:HG12	2.18	0.44
1:B:346:PRO:HD2	1:B:400:GLU:O	2.18	0.44
1:A:125:LYS:O	1:B:100:ARG:HB2	2.18	0.43
1:B:107:ALA:HA	1:B:153:PHE:O	2.19	0.43
1:A:185:ASN:HB3	1:A:205:TYR:CE2	2.54	0.43
1:A:230:TRP:CD2	1:A:237:LEU:HD13	2.54	0.43
1:B:193:PHE:HB2	1:B:334:LEU:CD2	2.50	0.42
1:B:159:ASN:HA	1:B:160:PRO:HA	1.78	0.42
1:B:145:ILE:HD11	1:B:152:ILE:HD11	2.03	0.41
1:B:353:ALA:HA	1:B:402:ILE:HD11	2.02	0.41
1:B:190:PRO:HA	1:B:193:PHE:O	2.21	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	400/433 (92%)	391 (98%)	9 (2%)	0	100	100
1	B	399/433 (92%)	388 (97%)	11 (3%)	0	100	100
All	All	799/866 (92%)	779 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	317/358 (88%)	313 (99%)	4 (1%)	61	77
1	B	304/358 (85%)	299 (98%)	5 (2%)	55	73
All	All	621/716 (87%)	612 (99%)	9 (1%)	57	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	MET
1	A	330	TYR
1	A	410	ASP
1	A	418	ILE
1	B	159	ASN
1	B	182	ILE
1	B	244	TYR
1	B	330	TYR

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Mol	Chain	Res	Type
1	B	366	LEU

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

Mol	Chain	Res	Type
1	B	159	ASN
1	B	368	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	LLP	A	209	1	23,24,25	0.47	0	25,32,34	0.63	0
1	LLP	B	209	1	23,24,25	0.46	0	25,32,34	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
1	LLP	A	209	1	-	4/16/17/19	0/1/1/1
1	LLP	B	209	1	-	8/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	209	LLP	C4-C4'-NZ-CE
1	A	209	LLP	O-C-CA-CB
1	B	209	LLP	C4-C4'-NZ-CE
1	B	209	LLP	C5'-OP4-P-OP2
1	B	209	LLP	C5'-OP4-P-OP3
1	B	209	LLP	O-C-CA-CB
1	B	209	LLP	CG-CD-CE-NZ
1	A	209	LLP	CG-CD-CE-NZ
1	B	209	LLP	C5'-OP4-P-OP1
1	B	209	LLP	CA-CB-CG-CD
1	A	209	LLP	C-CA-CB-CG
1	B	209	LLP	C3-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

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

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	405/433 (93%)	0.05	9 (2%) 62 64	24, 54, 81, 124	1 (0%)
1	B	402/433 (92%)	0.41	18 (4%) 38 40	26, 69, 101, 127	1 (0%)
All	All	807/866 (93%)	0.23	27 (3%) 49 51	24, 61, 93, 127	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	LEU	4.7
1	A	47	LEU	3.6
1	B	391	GLU	3.5
1	A	44	ALA	3.4
1	B	244	TYR	3.3
1	B	60	ILE	3.3
1	A	39	GLU	3.3
1	B	301	MET	3.0
1	B	388	THR	2.9
1	B	427	GLU	2.9
1	B	390	GLU	2.9
1	B	112	TYR	2.8
1	B	395	ALA	2.6
1	A	48	PHE	2.6
1	B	380	ALA	2.5
1	B	381	SER	2.4
1	A	301	MET	2.4
1	B	378	HIS	2.3
1	B	39	GLU	2.3
1	A	244	TYR	2.2
1	A	60	ILE	2.2
1	B	426	LEU	2.2
1	A	38	PHE	2.1
1	B	368	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	340	ALA	2.1
1	B	397	VAL	2.0
1	B	238	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	209	24/25	0.96	0.08	45,59,63,64	0
1	LLP	B	209	24/25	0.96	0.11	57,66,71,72	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.