



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 01:01 am BST

PDB ID : 6MLY  
Title : Bifunctional GH43-CE Bacteroides eggerthii, BACEGG\_01304  
Authors : Koropatkin, N.M.; Pereira, G.V.; Cann, I.  
Deposited on : 2018-09-28  
Resolution : 2.70 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

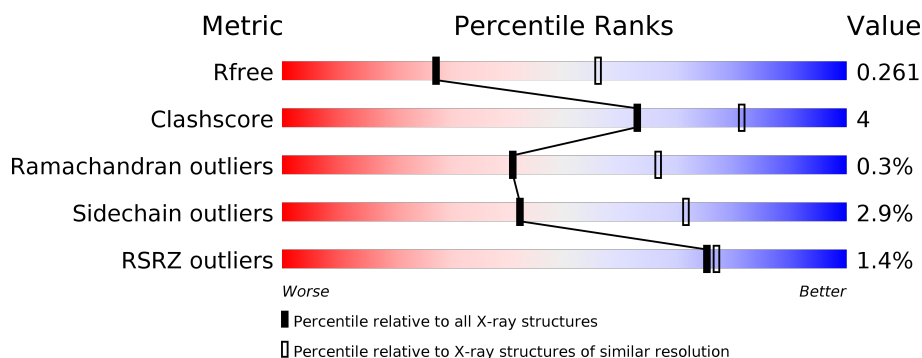
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	807	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>12%</div> </div> </div>
1	B	807	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	807	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>.</div> </div> </div>
1	D	807	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24144 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 Bifunctional GH43-CE protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5555	3570	925	1032	28			
1	B	772	Total	C	N	O	S	0	0	0
			6046	3871	1016	1128	31			
1	C	774	Total	C	N	O	S	0	0	0
			6051	3874	1018	1128	31			
1	D	772	Total	C	N	O	S	0	0	0
			6040	3869	1016	1124	31			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	expression tag	UNP A0A380YKU1
A	8	SER	-	expression tag	UNP A0A380YKU1
A	9	HIS	-	expression tag	UNP A0A380YKU1
A	10	MET	-	expression tag	UNP A0A380YKU1
A	11	ALA	-	expression tag	UNP A0A380YKU1
A	12	SER	-	expression tag	UNP A0A380YKU1
A	13	MET	-	expression tag	UNP A0A380YKU1
A	14	THR	-	expression tag	UNP A0A380YKU1
A	15	GLY	-	expression tag	UNP A0A380YKU1
A	16	GLY	-	expression tag	UNP A0A380YKU1
A	17	GLN	-	expression tag	UNP A0A380YKU1
A	18	GLN	-	expression tag	UNP A0A380YKU1
A	19	MET	-	expression tag	UNP A0A380YKU1
A	20	GLY	-	expression tag	UNP A0A380YKU1
A	21	ARG	-	expression tag	UNP A0A380YKU1
A	22	GLY	-	expression tag	UNP A0A380YKU1
A	23	SER	-	expression tag	UNP A0A380YKU1
A	798	TYR	-	expression tag	UNP A0A380YKU1
A	799	ARG	-	expression tag	UNP A0A380YKU1
A	800	ASP	-	expression tag	UNP A0A380YKU1
A	801	LEU	-	expression tag	UNP A0A380YKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	802	ASN	-	expression tag	UNP A0A380YKU1
A	803	ARG	-	expression tag	UNP A0A380YKU1
A	804	ILE	-	expression tag	UNP A0A380YKU1
A	805	ARG	-	expression tag	UNP A0A380YKU1
A	806	PRO	-	expression tag	UNP A0A380YKU1
A	807	ILE	-	expression tag	UNP A0A380YKU1
A	808	LYS	-	expression tag	UNP A0A380YKU1
A	809	CYS	-	expression tag	UNP A0A380YKU1
A	810	ASP	-	expression tag	UNP A0A380YKU1
A	811	ASP	-	expression tag	UNP A0A380YKU1
A	812	ILE	-	expression tag	UNP A0A380YKU1
A	813	LYS	-	expression tag	UNP A0A380YKU1
B	7	GLY	-	expression tag	UNP A0A380YKU1
B	8	SER	-	expression tag	UNP A0A380YKU1
B	9	HIS	-	expression tag	UNP A0A380YKU1
B	10	MET	-	expression tag	UNP A0A380YKU1
B	11	ALA	-	expression tag	UNP A0A380YKU1
B	12	SER	-	expression tag	UNP A0A380YKU1
B	13	MET	-	expression tag	UNP A0A380YKU1
B	14	THR	-	expression tag	UNP A0A380YKU1
B	15	GLY	-	expression tag	UNP A0A380YKU1
B	16	GLY	-	expression tag	UNP A0A380YKU1
B	17	GLN	-	expression tag	UNP A0A380YKU1
B	18	GLN	-	expression tag	UNP A0A380YKU1
B	19	MET	-	expression tag	UNP A0A380YKU1
B	20	GLY	-	expression tag	UNP A0A380YKU1
B	21	ARG	-	expression tag	UNP A0A380YKU1
B	22	GLY	-	expression tag	UNP A0A380YKU1
B	23	SER	-	expression tag	UNP A0A380YKU1
B	798	TYR	-	expression tag	UNP A0A380YKU1
B	799	ARG	-	expression tag	UNP A0A380YKU1
B	800	ASP	-	expression tag	UNP A0A380YKU1
B	801	LEU	-	expression tag	UNP A0A380YKU1
B	802	ASN	-	expression tag	UNP A0A380YKU1
B	803	ARG	-	expression tag	UNP A0A380YKU1
B	804	ILE	-	expression tag	UNP A0A380YKU1
B	805	ARG	-	expression tag	UNP A0A380YKU1
B	806	PRO	-	expression tag	UNP A0A380YKU1
B	807	ILE	-	expression tag	UNP A0A380YKU1
B	808	LYS	-	expression tag	UNP A0A380YKU1
B	809	CYS	-	expression tag	UNP A0A380YKU1
B	810	ASP	-	expression tag	UNP A0A380YKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	811	ASP	-	expression tag	UNP A0A380YKU1
B	812	ILE	-	expression tag	UNP A0A380YKU1
B	813	LYS	-	expression tag	UNP A0A380YKU1
C	7	GLY	-	expression tag	UNP A0A380YKU1
C	8	SER	-	expression tag	UNP A0A380YKU1
C	9	HIS	-	expression tag	UNP A0A380YKU1
C	10	MET	-	expression tag	UNP A0A380YKU1
C	11	ALA	-	expression tag	UNP A0A380YKU1
C	12	SER	-	expression tag	UNP A0A380YKU1
C	13	MET	-	expression tag	UNP A0A380YKU1
C	14	THR	-	expression tag	UNP A0A380YKU1
C	15	GLY	-	expression tag	UNP A0A380YKU1
C	16	GLY	-	expression tag	UNP A0A380YKU1
C	17	GLN	-	expression tag	UNP A0A380YKU1
C	18	GLN	-	expression tag	UNP A0A380YKU1
C	19	MET	-	expression tag	UNP A0A380YKU1
C	20	GLY	-	expression tag	UNP A0A380YKU1
C	21	ARG	-	expression tag	UNP A0A380YKU1
C	22	GLY	-	expression tag	UNP A0A380YKU1
C	23	SER	-	expression tag	UNP A0A380YKU1
C	798	TYR	-	expression tag	UNP A0A380YKU1
C	799	ARG	-	expression tag	UNP A0A380YKU1
C	800	ASP	-	expression tag	UNP A0A380YKU1
C	801	LEU	-	expression tag	UNP A0A380YKU1
C	802	ASN	-	expression tag	UNP A0A380YKU1
C	803	ARG	-	expression tag	UNP A0A380YKU1
C	804	ILE	-	expression tag	UNP A0A380YKU1
C	805	ARG	-	expression tag	UNP A0A380YKU1
C	806	PRO	-	expression tag	UNP A0A380YKU1
C	807	ILE	-	expression tag	UNP A0A380YKU1
C	808	LYS	-	expression tag	UNP A0A380YKU1
C	809	CYS	-	expression tag	UNP A0A380YKU1
C	810	ASP	-	expression tag	UNP A0A380YKU1
C	811	ASP	-	expression tag	UNP A0A380YKU1
C	812	ILE	-	expression tag	UNP A0A380YKU1
C	813	LYS	-	expression tag	UNP A0A380YKU1
D	7	GLY	-	expression tag	UNP A0A380YKU1
D	8	SER	-	expression tag	UNP A0A380YKU1
D	9	HIS	-	expression tag	UNP A0A380YKU1
D	10	MET	-	expression tag	UNP A0A380YKU1
D	11	ALA	-	expression tag	UNP A0A380YKU1
D	12	SER	-	expression tag	UNP A0A380YKU1

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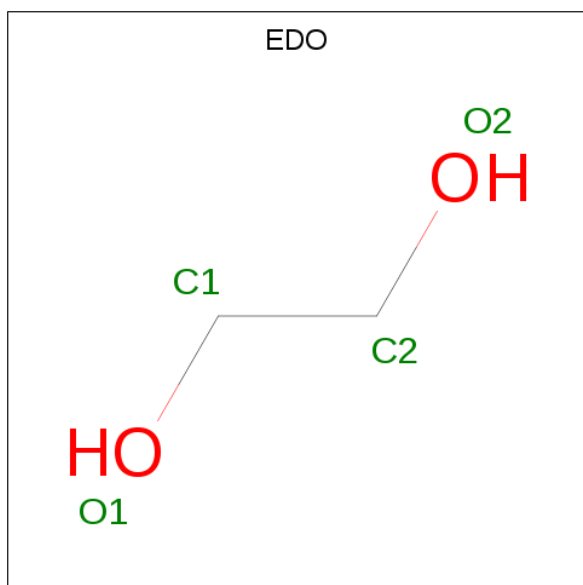
Chain	Residue	Modelled	Actual	Comment	Reference
D	13	MET	-	expression tag	UNP A0A380YKU1
D	14	THR	-	expression tag	UNP A0A380YKU1
D	15	GLY	-	expression tag	UNP A0A380YKU1
D	16	GLY	-	expression tag	UNP A0A380YKU1
D	17	GLN	-	expression tag	UNP A0A380YKU1
D	18	GLN	-	expression tag	UNP A0A380YKU1
D	19	MET	-	expression tag	UNP A0A380YKU1
D	20	GLY	-	expression tag	UNP A0A380YKU1
D	21	ARG	-	expression tag	UNP A0A380YKU1
D	22	GLY	-	expression tag	UNP A0A380YKU1
D	23	SER	-	expression tag	UNP A0A380YKU1
D	798	TYR	-	expression tag	UNP A0A380YKU1
D	799	ARG	-	expression tag	UNP A0A380YKU1
D	800	ASP	-	expression tag	UNP A0A380YKU1
D	801	LEU	-	expression tag	UNP A0A380YKU1
D	802	ASN	-	expression tag	UNP A0A380YKU1
D	803	ARG	-	expression tag	UNP A0A380YKU1
D	804	ILE	-	expression tag	UNP A0A380YKU1
D	805	ARG	-	expression tag	UNP A0A380YKU1
D	806	PRO	-	expression tag	UNP A0A380YKU1
D	807	ILE	-	expression tag	UNP A0A380YKU1
D	808	LYS	-	expression tag	UNP A0A380YKU1
D	809	CYS	-	expression tag	UNP A0A380YKU1
D	810	ASP	-	expression tag	UNP A0A380YKU1
D	811	ASP	-	expression tag	UNP A0A380YKU1
D	812	ILE	-	expression tag	UNP A0A380YKU1
D	813	LYS	-	expression tag	UNP A0A380YKU1

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is water.

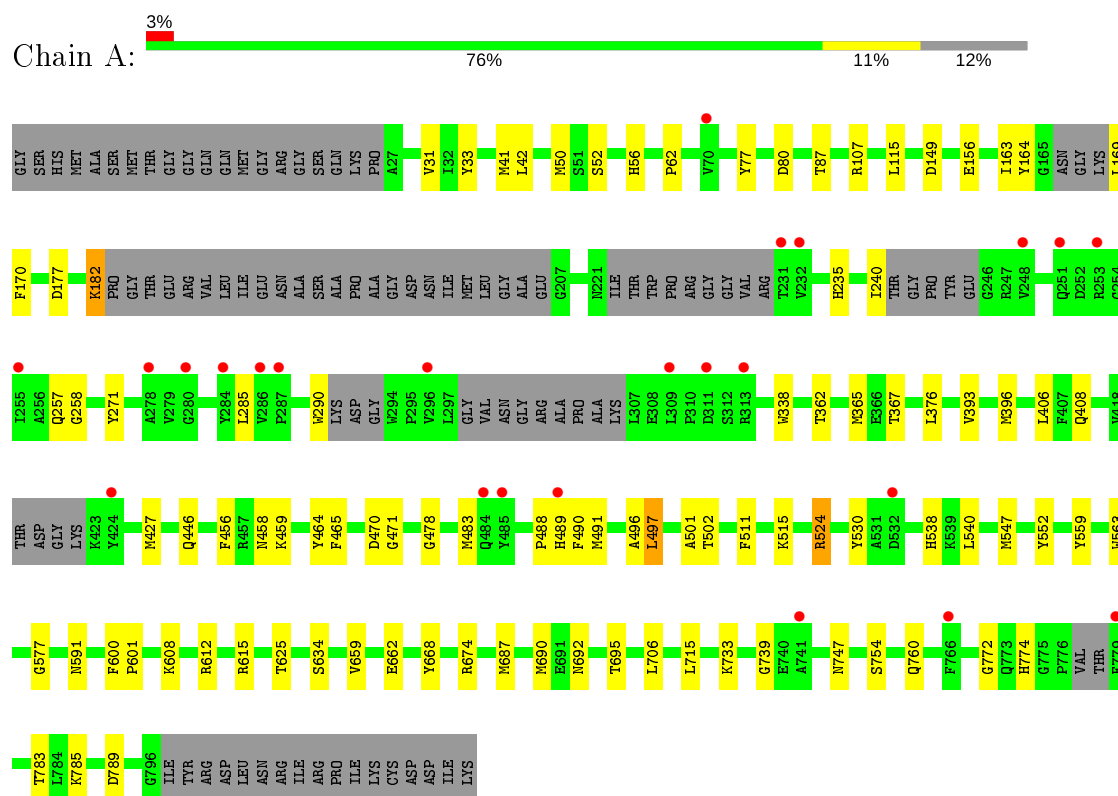
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	58	Total O 58 58	0	0
5	B	134	Total O 134 134	0	0
5	C	92	Total O 92 92	0	0
5	D	112	Total O 112 112	0	0



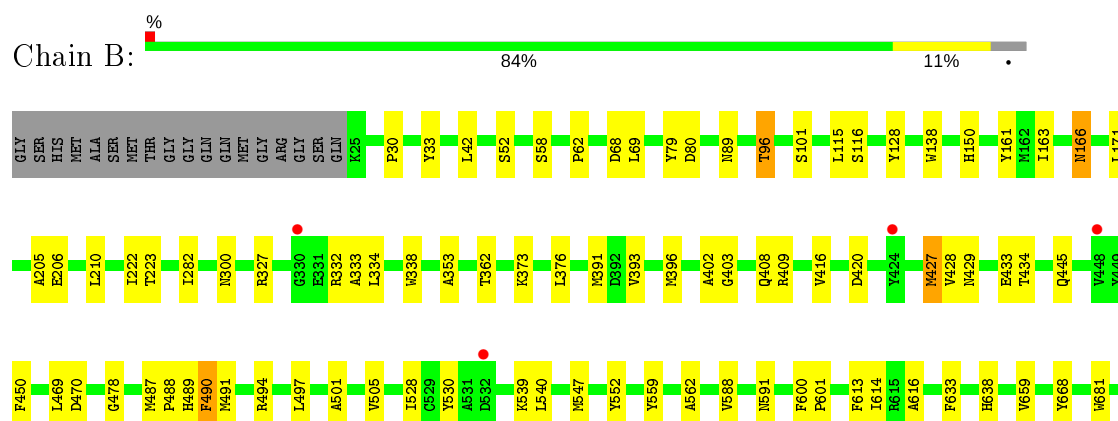
### 3 Residue-property plots [i](#)

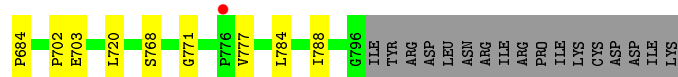
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Bifunctional GH43-CE protein

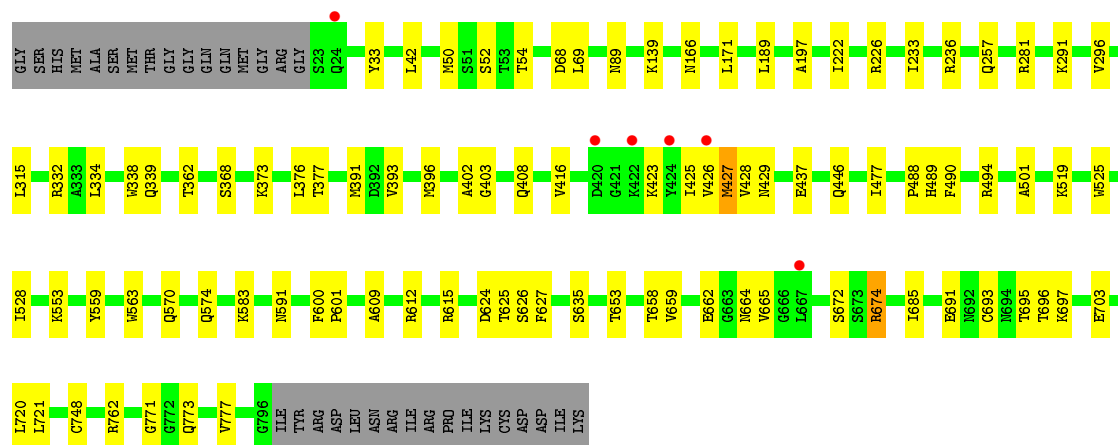
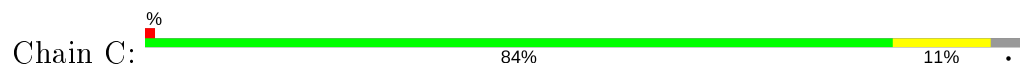


#### • Molecule 1: Bifunctional GH43-CE protein

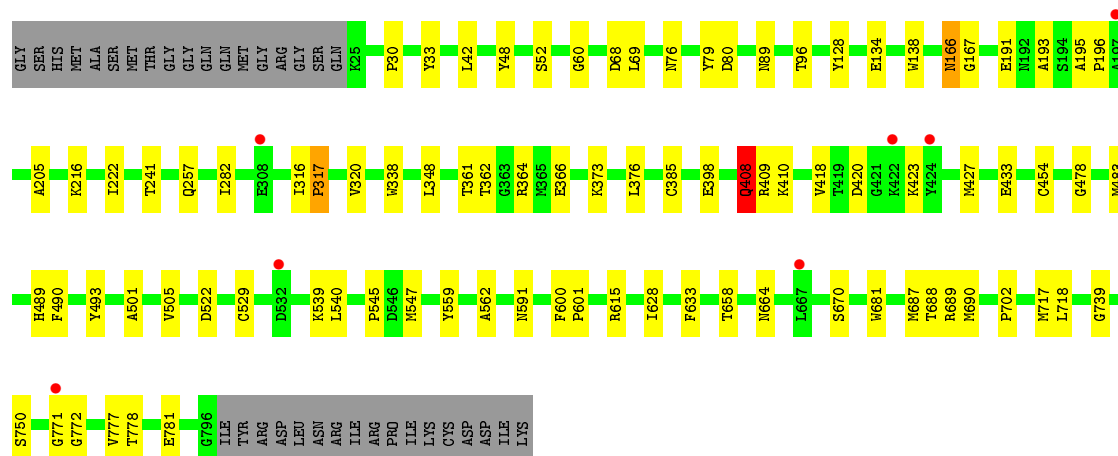
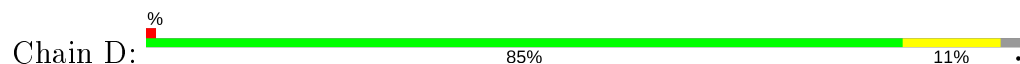




• Molecule 1: Bifunctional GH43-CE protein



• Molecule 1: Bifunctional GH43-CE protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	254.73Å 93.31Å 214.04Å 90.00° 123.38° 90.00°	Depositor
Resolution (Å)	48.16 – 2.70 48.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.16-2.70) 98.8 (48.12-2.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.220 , 0.269 0.211 , 0.261	Depositor DCC
$R_{free}$ test set	5719 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	1.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, EDO, ACT

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	0.53	6/5696 (0.1%)	0.57	2/7723 (0.0%)
1	B	0.34	0/6204	0.56	0/8413
1	C	0.34	0/6209	0.56	0/8421
1	D	0.34	0/6198	0.56	0/8405
All	All	0.40	6/24307 (0.0%)	0.56	2/32962 (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	B	0	2
1	C	0	2
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	LYS	C-O	21.93	1.65	1.23
1	A	240	ILE	C-O	15.81	1.53	1.23
1	A	290	TRP	C-O	9.35	1.41	1.23
1	A	524	ARG	NE-CZ	5.65	1.40	1.33
1	A	107	ARG	NE-CZ	5.31	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	A	107	ARG	NE-CZ-NH1	6.35	123.47	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	ASN	Peptide
1	B	494	ARG	Sidechain
1	C	236	ARG	Sidechain
1	C	762	ARG	Sidechain

## 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	5555	0	5337	47	0
1	B	6046	0	5888	56	0
1	C	6051	0	5888	52	0
1	D	6040	0	5884	48	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	8	0	12	1	0
3	B	4	0	6	0	0
3	C	8	0	12	2	0
3	D	16	0	24	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	58	0	0	0	0
5	B	134	0	0	0	0
5	C	92	0	0	0	0
5	D	112	0	0	2	0
All	All	24144	0	23063	202	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 4.

The worst 5 of 202 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:182:LYS:C	1:A:182:LYS:O	1.65	1.33
1:A:612:ARG:HH12	1:A:662:GLU:HG2	1.40	0.87
1:A:612:ARG:NH1	1:A:662:GLU:HG2	1.95	0.81
1:B:408:GLN:HG2	1:B:409:ARG:H	1.48	0.79
1:C:570:GLN:HE21	1:C:574:GLN:HE21	1.33	0.74

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	693/807 (86%)	645 (93%)	45 (6%)	3 (0%)	34	60
1	B	770/807 (95%)	719 (93%)	50 (6%)	1 (0%)	51	78
1	C	772/807 (96%)	722 (94%)	49 (6%)	1 (0%)	51	78
1	D	770/807 (95%)	719 (93%)	48 (6%)	3 (0%)	34	60
All	All	3005/3228 (93%)	2805 (93%)	192 (6%)	8 (0%)	41	66

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	577	GLY
1	A	747	ASN
1	D	408	GLN
1	C	257	GLN
1	D	257	GLN

### 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	581/669 (87%)	562 (97%)	19 (3%)	38	67
1	B	639/669 (96%)	624 (98%)	15 (2%)	50	78
1	C	638/669 (95%)	619 (97%)	19 (3%)	41	70
1	D	637/669 (95%)	618 (97%)	19 (3%)	41	70
All	All	2495/2676 (93%)	2423 (97%)	72 (3%)	42	71

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	703	GLU
1	C	226	ARG
1	D	670	SER
1	B	768	SER
1	C	52	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	339	GLN
1	D	413	GLN
1	C	446	GLN
1	A	570	GLN
1	C	339	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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	$\# Z  > 2$
3	EDO	D	905	-	3,3,3	0.51	0	2,2,2	0.02	0
2	ACT	B	901	-	1,3,3	1.21	0	0,3,3	0.00	-
2	ACT	C	901	-	1,3,3	1.42	0	0,3,3	0.00	-
2	ACT	A	901	-	1,3,3	1.67	0	0,3,3	0.00	-
3	EDO	D	902	-	3,3,3	0.59	0	2,2,2	0.19	0
3	EDO	C	903	-	3,3,3	0.53	0	2,2,2	0.11	0
3	EDO	D	903	-	3,3,3	0.73	0	2,2,2	0.21	0
3	EDO	A	903	-	3,3,3	0.40	0	2,2,2	0.30	0
3	EDO	A	902	-	3,3,3	0.46	0	2,2,2	0.44	0
3	EDO	D	904	-	3,3,3	0.54	0	2,2,2	0.12	0
3	EDO	B	902	-	3,3,3	0.50	0	2,2,2	0.20	0
3	EDO	C	902	-	3,3,3	0.55	0	2,2,2	0.07	0
2	ACT	D	901	-	1,3,3	1.22	0	0,3,3	0.00	-

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
3	EDO	D	905	-	-	0/1/1/1	-
3	EDO	B	902	-	-	1/1/1/1	-
3	EDO	D	902	-	-	1/1/1/1	-
3	EDO	C	903	-	-	1/1/1/1	-
3	EDO	D	903	-	-	1/1/1/1	-
3	EDO	A	903	-	-	1/1/1/1	-
3	EDO	A	902	-	-	0/1/1/1	-
3	EDO	D	904	-	-	0/1/1/1	-
3	EDO	C	902	-	-	1/1/1/1	-

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	EDO	O1-C1-C2-O2
3	D	903	EDO	O1-C1-C2-O2
3	D	902	EDO	O1-C1-C2-O2
3	C	903	EDO	O1-C1-C2-O2
3	B	902	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	905	EDO	1	0
3	A	903	EDO	1	0
3	C	902	EDO	2	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	711/807 (88%)	0.09	24 (3%) 45 45	61, 77, 93, 111	0
1	B	772/807 (95%)	-0.29	5 (0%) 89 91	44, 56, 71, 87	0
1	C	774/807 (95%)	-0.20	6 (0%) 86 87	49, 63, 77, 96	0
1	D	772/807 (95%)	-0.17	7 (0%) 84 85	46, 61, 79, 93	0
All	All	3029/3228 (93%)	-0.15	42 (1%) 75 77	44, 63, 84, 111	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	VAL	4.5
1	D	424	TYR	3.6
1	A	424	TYR	3.6
1	A	251	GLN	3.6
1	D	667	LEU	3.3

### 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 carbohydrates in this entry.

### 6.4 Ligands [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, 95<sup>th</sup> 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
3	EDO	D	904	4/4	0.80	0.17	55,57,59,61	0
3	EDO	C	902	4/4	0.87	0.28	55,55,60,64	0
3	EDO	D	903	4/4	0.89	0.15	75,77,84,92	0
3	EDO	D	905	4/4	0.89	0.27	62,64,70,71	0
3	EDO	D	902	4/4	0.89	0.24	65,68,71,72	0
3	EDO	A	902	4/4	0.90	0.20	59,65,70,76	0
4	NA	D	906	1/1	0.91	0.25	37,37,37,37	0
3	EDO	A	903	4/4	0.93	0.20	44,47,51,52	0
3	EDO	B	902	4/4	0.95	0.15	59,62,62,63	0
4	NA	A	904	1/1	0.95	0.27	40,40,40,40	0
3	EDO	C	903	4/4	0.96	0.11	46,49,52,58	0
4	NA	C	904	1/1	0.97	0.20	43,43,43,43	0
2	ACT	A	901	4/4	0.97	0.07	47,49,50,59	0
2	ACT	C	901	4/4	0.97	0.12	48,49,50,50	0
4	NA	B	903	1/1	0.98	0.43	60,60,60,60	0
2	ACT	B	901	4/4	0.98	0.18	42,46,46,48	0
2	ACT	D	901	4/4	0.98	0.15	46,48,49,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.